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**Efficient Numerical Methods for Fractional Differential Equations
and their Analytical Background**

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Introduction

It seems like one day very useful consequences will be drawn from this paradox, since there are little paradoxes without usefulness. Leibniz in a letter [117] to L'Hospital on the significance of derivatives of order $1/2$.

Fractional Calculus

The field of fractional calculus is almost as old as calculus itself, but over the last decades the usefulness of this mathematical theory in applications as well as its merits in pure mathematics has become more and more evident. Recently a number of textbooks [105, 110, 122, 141] have been published on this field dealing with various aspects in different ways. Possibly the easiest access to the idea of the non-integer differential and integral operators studied in the field of fractional calculus is given by Cauchy's well known representation of an n -fold integral as a convolution integral

$$\begin{aligned} J^n y(x) &= \int_0^x \int_0^{x_{n-1}} \cdots \int_0^{x_1} y(x_0) dx_0 \cdots dx_{n-2} dx_{n-1} \\ &= \frac{1}{(n-1)!} \int_0^x \frac{1}{(x-t)^{1-n}} y(t) dt, \quad n \in \mathbb{N}, x \in \mathbb{R}_+, \end{aligned}$$

where J^n is the n -fold integral operator with $J^0 y(x) = y(x)$. Replacing the discrete factorial $(n-1)!$ with Euler's continuous gamma function $\Gamma(n)$, which satisfies $(n-1)! = \Gamma(n)$ for $n \in \mathbb{N}$, one obtains a definition of a non-integer order integral, i.e.

$$J^\alpha y(x) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{1}{(x-t)^{1-\alpha}} y(t) dt, \quad \alpha, x \in \mathbb{R}_+.$$

Several important aspects of fractional calculus originate from non-integer order derivatives, which can simplest be defined as concatenation of integer order differentiation and fractional integration, i.e.

$$D^\alpha y(x) = D^n J^{n-\alpha} y(x) \quad \text{or} \quad D_*^\alpha y(x) = J^{n-\alpha} D^n y(x),$$

where n is the integer satisfying $\alpha \leq n < \alpha + 1$ and D^n , $n \in \mathbb{N}$, is the n -fold differential operator with $D^0 y(x) = y(x)$. The operator D^α is usually denoted as *Riemann-Liouville*

differential operator, while the operator D_*^α is named *Caputo differential operator*. The fact that there is obviously more than one way to define non-integer order derivatives is one of the challenging and rewarding aspects of this mathematical field.

Because of the integral in the definition of the non-integer order derivatives, it is apparent that these derivatives are non-local operators, which explains one of their most significant uses in applications: A non-integer derivative at a certain point in time or space contains information about the function at earlier points in time or space respectively. Thus non-integer derivatives possess a memory effect, which it shares with several materials such as viscoelastic materials or polymers as well as principles in applications such as anomalous diffusion. This fact is also one of the reasons for the recent interest in fractional calculus: Because of their non-local property fractional derivatives can be used to construct *simple* material models and unified principles. Prominent examples for diffusion processes are given in the textbook by Oldham and Spanier [110] and the paper by Olmstead and Handelsman [111], examples for modeling viscoelastic materials can be found in the classic papers of Bagley and Torvik [10], Caputo [20], and Caputo and Mainardi [21] and applications in the field of signal processing are discussed in the publication [104] by Marks and Hall. Several newer results can be found e.g. in the works of Chern [24], Diethelm and Freed [39], Gaul, Klein and Kempfle [57], Unser and Blu [143, 144], Podlubny [121] and Podlubny et. al [124]. Additionally a number of surveys with collections of applications can be found e.g. in Gorenflo and Mainardi [59], Mainardi [102] or Podlubny [122].

The utilization of the memory effect of fractional derivatives in the construction of simple material models or unified principles comes with a high cost regarding numerical solvability. Any algorithm using a discretization of a non-integer derivative has, among other things, to take into account its non-local structure which means in general a high storage requirement and great overall complexity of the algorithm. Numerous attempts to solve equations involving different types of non-integer order operators can be found in the literature: Several articles by Brunner [14, 15, 16, 17, 18] deal with so-called collocation methods to solve Abel-Volterra integral equations. In these equations the integral part is essentially the non-integer order integral as defined above. These, and additional results can also be found in his book [19] on this topic. A book [83] by Linz and an article by Orsi [112] e.g. use product integration techniques to solve Abel-Volterra integral equations as well. Several articles by Lubich [92, 93, 94, 95, 96, 98], and Hairer, Lubich and Schlichte [63], use so called fractional linear multistep methods to solve Abel-Volterra integral equations numerically. In addition several papers deal with numerical methods to solve differential equations of fractional order. These equations are similar to ordinary differential equations, with the exception that the derivatives occurring in them are of non-integer order. Approaches based on fractional formulation of backward difference methods can e.g. be found in the papers by Diethelm [31, 38, 42], Ford and Simpson [53, 54, 55], Podlubny [123] and Walz [146]. Fractional formulation of Adams-type methods are e.g. discussed in the papers [36, 37] by Diethelm et al. Except the collocation methods by Brunner and the product integration techniques by Linz and Orsi, most of the cited ideas are presented and advanced in this thesis.

Outline of the thesis

In this thesis several aspects of fractional calculus will be presented ranging from its history over analytical and numerical results to applications. The structure of this thesis is deliberately chosen in such a way that not only experts in the field of fractional calculus can understand the presented results within this thesis, but also readers with knowledge obtained e.g. in the first semesters of a mathematical or engineering study course can comprehend the benefits and the problems of *efficient numerical methods for fractional differential equations and their analytical background*. For this reason this thesis is structured as follows:

The thesis begins in Chapter 1 with a brief historical review of the theory of fractional calculus and its applications. The theory of non-integer order differentiation and integration is almost as old as classical calculus itself, but nevertheless there seems to be an astonishing lack of knowledge of this field in most mathematicians. A look at the historical development can in parts explain the absence of this field in today's standard mathematics textbooks on calculus and in addition give the reader not familiar with this field a good access to the topics addressed in this thesis. Moreover, the possession of an understanding of the historical development of any mathematical field often can give significant additional insight in an otherwise only theoretical presentation.

In Chapter 2 some well known analytical and numerical results on classical calculus are stated. One reason behind this is due to the fact that those results are needed for several proofs of theorems in later chapters and thus they are stated here for completeness. Moreover, classical calculus can be regarded as a special case of fractional calculus, since results in fractional calculus should contain the classical case in a certain way. Therefore, the results presented in Chapter 2 can also be viewed as control results for the findings presented in the later chapters of this thesis.

Chapter 3 also states some well known results on integral transforms and special functions. The results of that chapter will be used frequently in the succeeding chapters dealing with the analytical and numerical theory of fractional calculus.

Analytical results of fractional calculus and in particular differential equations of fractional order are presented in Chapter 4. Most of the stated results can be found in similar form in textbooks on fractional calculus, but some of the presented results give additional properties or corrected statements of known theorems as well. The analytical properties of fractional calculus build the fundament of any numerical methods for differential equations of fractional order. Thus, rigorous proofs are given for most theorems in order to motivate and warrant the numerical methods for such differential equations, which are presented in the succeeding chapter.

Numerical methods are presented in Chapter 5. In parts they provide a deeper understanding of known methods developed over the last decades and in addition some new methods are presented. One important aspect in Chapter 5 is a careful survey of the possible implementation of some of the presented methods in computer algorithms. While this seems on a first glance less of a mathematical problem than a problem to be dealt with in computer science it will be shown mathematically that some of the presented methods may lead to completely wrong numerical results in any of today's used implementations. Therefore, Chapter 5 gives the reader an extensive overview of known and new numerical methods for fractional differential equations available today and in addition points out the

aspects which have to be handled with care in their implementation.

In Chapter 6 the presented numerical methods are tested for several test equations and the theoretical results of Chapter 5 are verified. In addition some of the numerical methods are extended to deal with partial differential equations of fractional order. Finally an application from physics/chemistry is presented and it is shown which pitfalls need to be overcome to successfully apply some of the presented methods. The thesis finishes in Chapter 7 with a conclusion of the covered aspects of fractional calculus.

New results

Since this thesis is structured more as a textbook than a showcase of the new results produced by the author, the new findings of this thesis are briefly summarized in Chapter 7 so that experts on the mathematical field of fractional calculus may check there first. Additionally the chapters containing new and important analytical and numerical results are pointed out below:

In Chapter 4.2.1 the smoothness properties of the solution of Abel-Volterra equations are developed. This kind of equations are tightly connected with fractional order differential equations as shown e.g. in Chapter 4.2. Lubich [94], and Miller and Feldstein [107] provided a very detailed analysis of the smoothness properties of the solution of Abel-Volterra integral equations, which in parts has some minor, but important errors in it. In Chapter 4.2.1 these errors are corrected and interesting consequences are drawn from the corrected theorems.

The whole Chapter 5 is devoted to a rather extensive review of numerical algorithms for differential equations of fractional order. While the stated results are often not new, some minor errors in their implementation are found every now and then in recent articles. Therefore, these common methods are rigorously restated in this chapter. However, a more important new result presented within this chapter is given by a careful analysis of higher-order backward difference methods, which are based on several papers by Lubich [93, 95, 96, 97] and Hairer, Lubich and Schlichte [63], where fractional linear multistep methods are developed and implemented for Abel-Volterra integral equations. This analysis, carried out for, but not restricted to fractional order differential equations, is given in Chapter 5.1.3. The result of this analysis is disillusioning in the sense, that in general higher-order backward methods simply will not work properly in any implementation, unless severe restrictions are applied e.g. on the order of the differential equation. But a remedy of this situation is also contained within this thesis, mainly based on results presented in Chapter 5.2. There two methods to compute the exact expansion of the analytic solution of fractional order differential equations are presented. With the knowledge of such an expansion the problems presented in Chapter 5.1.3 can be reduced or even prevented. Numerical examples verifying these findings are given in Chapter 6.1.

An expansion of the presented numerical methods for fractional order differential equations to partial differential equations of fractional order is presented in Chapter 6.2. The given ideas take into account the general structure of fractional derivatives and apply different fractional order backward difference methods to construct a new solver for time-fractional diffusion-wave equations.

Finally in Chapter 6.3 a new approach to handle a flame propagation model by Joulin [74] numerically is presented and its advantages over other recently presented approaches [8, 9, 46, 74] are pointed out.

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Marc Weilbeer, January 2005

Chapter 1

A brief history of fractional calculus

During the last decades *fractional calculus* has blossomed and grown in pure mathematics as well as in scientific applications. But to classify fractional calculus as a young science would be utterly wrong. In fact, the origin of fractional calculus lies nearly as far back as classical calculus itself. On the other hand today's mathematical topics which fall under the class of fractional calculus are far from being the “calculus of fractions” as one might suspect by the notation itself. Instead, *integration and differentiation to an arbitrary order* would be a better notation for the field of fractional calculus as it is understood today. Both the age of fractional calculus and the fact that *fractional calculus* itself is a misnomer in its use today can be explained by surveying some aspects of the history of this mathematical field. Therefore, the beginning of this work is concerned with a short summarization of the history of fractional calculus.

In recent years a number of books [105, 110, 122, 141] on fractional calculus were published and in all of them its history is addressed in one way or another. Additionally a number of papers [134, 135, 136, 137] by Ross deal with various aspects of the history of fractional calculus.

In this chapter we divide the historical retrospection into three sections each representing a stage in the development of fractional calculus. However, the coarse partition in only three stages could be subdivided much finer but the scope of this chapter is to give an overview of the historical development rather than a complete survey of the history of fractional calculus.

1.1 The early stages 1695-1822

While the birth of classical calculus is associated with Leibniz and Newton and in fact, is a historical controversy by itself (see e.g. [66]), the origin of fractional calculus can be traced back to Leibniz alone, more precise to his notation $d^n y/dx^n$ for the n th derivative of a function $y(x)$, where n is supposed to be an integer. While there are no mathematical scripts from Leibniz on derivatives of non-integer order, there are a number of letters sent from

and to him which mention such derivatives and address their mathematical merits. However, most of these early results and conjectures are not used in today's theory of fractional calculus. For this reason the point of view in this first section of the historical outline shifts from the mathematical to a more historical one. This means that in this chapter passages in letters and papers are completely quoted in translation and some important aspects of them get pointed out¹. In the later sections of this chapter a more mathematical approach will be carried out, taking the greater impact on today's theory of fractional calculus into account.

One of the earliest remarks on the meaning on non-integer derivatives can be found in a letter [117] from Leibniz to L'Hospital dated 3.8.1695, where Leibniz gives a first answer to a question posed by L'Hospital about the meaning of non-integer derivatives, especially the case $1/2$. In his letter Leibniz writes:

“You can see here sir, that one can express a term like $d^{\frac{1}{2}}\overline{xy}$ or $d^{1:2}\overline{xy}$ by an infinite series, even though it seems to be far from the geometry, which usually only considers the differences of positive integer exponents or the negatives with respect to sums, but not yet those, whose exponents are fractional. It is true that it is still to show that it is this series for $d^{1:2}x$; but not only this can be explained in a way. Because the ordinates x are expressed in a geometric series, such that by choosing a constant $d\beta$ it follows that $dx = xd\beta : a$, or (if one chose a as unit) $dx = xd\beta$, meaning ddx would be $x.\overline{d\beta}^2$, and d^3x would be $x.\overline{d\beta}^3$ etc. and $d^ex = x.\overline{d\beta}^e$. And thus the differential exponent has been changed by the exponents and by replacing $d\beta$ with $dx : x$, yielding $d^ex = \overline{dx : x}^e.x$. Thus it follows that $d^{\frac{1}{2}}x$ will be equal to $x\sqrt[2]{dx : x}$. It seems like one day very useful consequences will be drawn from this paradox, since there are little paradoxes without usefulness.”

Leibniz acknowledges the question raised by L'Hospital, considers its implications in mathematical terms “Thus it follows that $d^{\frac{1}{2}}x$ will be equal to $x\sqrt[2]{dx : x}$ ” and produces a conclusion by writing that “one day very useful consequences will be drawn from this paradox, since there are little paradoxes without usefulness.”. The topic of non-integer order derivatives also comes up in the correspondence between Johann Bernoulli and Leibniz. In a letter written to Leibniz in December 1695 Bernoulli reiterates the problem of “fractional or irrational” derivatives: [118]

“From the analogy you have shown that exponentiating and differentiating can easily be transferred to series for $d^m\overline{xy}$. If for the time being m denotes a fractional or irrational number, can you please explain to me what $d^m\overline{xy}$ would be, a quantity or something else? [...]”

Leibniz addresses this problem in a letter [119] back to Johann Bernoulli written in the same month, where he mentions derivatives of “general order” and repeats that issue in more detail compared to the letter to L'Hospital:

¹The translations of the quotes are done with care, but because of the author's limited knowledge of the original languages, which they were written in, mistakes in the given translations are inevitable. For this reason the reader can find the quoted passages in their original languages in Appendix C.

“What you are looking for in the derivatives, whose exponent is fractional or irrational, have I already considered in a letter to L’Hospital, and even though I have added this, the so structured derivatives can be compared with the ordinary ones. Let for example $d^{1:2}x$ be the proposed derivative. Let further x be an geometric progression. Let the assumed derivative constant be dh , and we have $xdh : a = dx$, and we get $d^2x = dxdh : a = xdhdh : aa$ and similarly $d^3x = xdh^3 : a^3$, and more general $d^ex = xdh^e : a^e$, as well as $d^{1:2}x = xdh^{1:2} : a^{1:2}$, or $d^{1:2}x = x\sqrt{dh} : a$ (here $1 : 2$ is the same as $\frac{1}{2}$; and $dh : a$ the same as $\frac{dh}{a}$). Thus you can see that such structured derivatives only have meaning by extracting the roots or by exponentiating of ordinary derivatives. I think this is memorable and you will not be unthankful for it. You have seen that the extra ordinary derivatives can be expressed by composing infinite geometric series and I suspect, that this will hold true for those cases which are not real.”

The last reference of fractional calculus during the lifetime of Leibniz can be found in one of his letters to J. Wallis in 1697 [120]. In the discussion of Wallis’ infinite product for $\pi/2$, Leibniz points out that differential calculus could have been used to achieve this result:

“At first glance my conclusion was that differentiation and summation in series with regards to derivatives and squaring correspond to each other. I discovered, that in geometry differences in differentiating are posed and noticed the delightful analogy of the relations between differences and sums and the relations between exponentiating and extracting roots. And I revealed that apart from the known properties of $y, y^2, y^3, y^{\frac{1}{2}}, y^{\frac{1}{3}}$ etc., or more general y^e , or $\boxed{p^e}y$, or exactly those powers of y with exponent e , the new form of differentiating or the changing states dy, d^2y (or ddy), d^3y (or ddy), can also be called in for $d^{\frac{1}{2}}y$, and more general d^ey .”

With the death of Leibniz in 1716 the topic of non-integer order derivatives did not end. It was Leonhard Euler, who in a paper [52] in 1783 worked on progressions of numbers and for the first time introduced the Gamma function as generalization of factorials, who pointed out in a small paragraph near the end of his paper:

“27. To round off this discussion, let me add something which certainly is more curious than useful. It is known that d^nx denotes the differential of x of order n , and if p denotes any function of x and dx is taken to be constant, then d^np is homogeneous with dx^n ; but whenever n is a positive whole number, the ratio of d^np to dx^n can be expressed algebraically; for example, if $n = 2$ and $p = x^3$, then $d^2(x^3)$ is to dx^2 as $6x$ to 1. We now ask, if n is a fractional number, what the value of that ratio should be. It is easy to understand the difficulty in this case; for if n is a positive whole number, d^n can be found by continued differentiation; such an approach is not available if n is a fractional number. But it will nevertheless be possible to disentangle the matter by using interpolation in progressions, which I have discussed in this essay.”

A bit over half a century after the death of Leibniz, the work of J.L. Lagrange indirectly contributed to the field of fractional calculus. In 1772 [77] Lagrange developed the law of

exponents for differential operators of integer order

$$\frac{d^m}{dx^m} \frac{d^n}{dx^n} = \frac{d^{m+n}}{dx^{m+n}}, \quad m, n \in \mathbb{N}.$$

This result can be transferred to arbitrary choices of $n, m \in \mathbb{C}$ under certain conditions (see further Chapter 4.1.1), which became evident much later in history.

Probably the first detailed definition of a fractional derivative is stated 1812 by P. S. Laplace in his book “Théorie analytique des probabilités” [78]. On a few pages Laplace defines a fractional derivative for functions representable by an integral $\int T(t)t^{-x}dt$:

“In order to clarify this, we consider the equation

$$y_x = \int T \cdot dt \cdot t^{-x},$$

where T is a function of t and the integral is evaluated on a given interval. Let x be a “variant” of α

$$\Delta \cdot y_x = \int T \cdot dt \cdot t^{-x} \cdot \left(\frac{1}{t^\alpha} - 1 \right)$$

or in general

$$\Delta^i \cdot y_x = \int T \cdot dt \cdot t^{-x} \cdot \left(\frac{1}{t^\alpha} - 1 \right)^i;$$

by choosing i to be negative, the symbol Δ in the integral changes the integral sign Σ . If α is infinite small and equals dx one gets $\frac{1}{t} = 1 + dx \cdot \log \cdot \frac{1}{t}$; Thus with the observation that $\Delta^i \cdot y_x$ changes to $d^i y_x$ one gets

$$\frac{d^i y_x}{dx^i} = \int T \cdot dt \cdot t^{-x} \cdot \left(\log \frac{1}{t} \right)^i.$$

In the same manner one gets by adopting the notation of n° 2

$$\nabla^i \cdot y_x = \int T \cdot dt \cdot t^{-x} \cdot \left(a + \frac{b}{t} \dots + \frac{q}{t^n} \right)^i.$$

Thus the same analysis, which results in successful derivation of the variables of the generating functions, gives the functions under the \int , the definite integral, expressing these derivatives. The symbol ∇^i expresses strictly speaking only a set i , containing consecutive operations. The examination of the generating functions reduces these operations to increasing a polynomial in its exponents; and the examination of the definite integrals yields directly the expression $\nabla^i \cdot y_x$, even in the case that i is a fractional number.

Laplace returns to fractional derivatives a bit later in the same book, where he generalizes his results to another set of functions:

“If the function y_s , dependent on s , can be represented by an integral of the form $\int x^s \cdot \varphi dx$, the infinitesimal differences of arbitrary order n are given by n° 21 as

$$\begin{aligned}\frac{d^n \cdot y_s}{ds^n} &= \int x^s \cdot \varphi dx \cdot (\log x)^n, \\ \Delta^n \cdot y_s &= \int x^s \cdot \varphi dx \cdot (x - 1)^n.\end{aligned}$$

If instead of representing the function of s as integral $\int x^s \cdot \varphi dx$, one uses the representation $\int c^{-sx} \cdot \varphi dx$, one gets accordingly

$$\begin{aligned}\frac{d^n \cdot y_s}{ds^n} &= (-1)^n \cdot \int x^n \cdot \varphi dx \cdot c^{-sx}, \\ \Delta^n \cdot y_s &= \int \varphi dx \cdot c^{-sx} \cdot (c^{-x} - 1)^n.\end{aligned}$$

In order to obtain negative integrals, which are assumed to be finite and infinitesimal, it is sufficient to choose n negative in the above formulas. One can ascertain that the formula holds even for general n , even if its a fraction.”

A couple of years later S. F. Lacroix also worked with fractional derivatives. Lacroix dedicates only two pages in an over 700 pages strong book [76] to work out the generalization of an integer order derivative of the function $y(x) = x^m$, $m \in \mathbb{N}$ to fractional order:

“Utilizing definite integrals, Euler succeeds again at a remarkable interpolation, the one of differential functions. Just as in between integer powers, by extracting the roots, one can use fractional powers to even understand the terms in between the series

$$V, \quad dV, \quad d^2V, \quad d^3V, \dots, d^nV,$$

the derivatives of the given function and its terms can be determined by a fractional number, which characterize the order in which it is used in the above series. It is neither possible to evaluate these parameters by successive differentiation, nor is it possible to explain the fractional powers by repeating multiplication; But the formulas $d^{\frac{1}{2}}V$ and $V^{\frac{1}{2}}$ will be formal expressions, one in the series of derivatives, the other one in the series of powers.

For example let $V = v^m$; If n is an integer number one obtains of arbitrary m ,

$$d^n(v^m) = m(m-1) \dots (m-n+1)v^{m-n}dv^n = \frac{[m]^m}{[m-n]^{m-n}}v^{m-n}dv^n;$$

setting for $[m]^m$ and $[m-n]^{m-n}$ the expressions of n° 1160, one obtains

$$d^n(v^m) = v^{m-n}dv^n \frac{\int dx(1/\frac{1}{x})^m}{\int dx(1/\frac{1}{x})^{m-n}}.$$

This result can immediately be verified; given that this formula contains the case, which is known, i.e. where n is a positive integer.

Setting $m = 1$ and $n = \frac{1}{2}$ one gets

$$d^{\frac{1}{2}}v = \sqrt{v}dv \frac{\int dx 1 \frac{1}{x}}{\int dx (1 \frac{1}{x})^{\frac{1}{2}}} = \frac{\sqrt{v}dv}{\frac{1}{2}\sqrt{\pi}},$$

and by the limits 0 and 1,

$$\int dx 1 \frac{1}{x} = 1, \quad \int dx \left(1 \frac{1}{x}\right)^{\frac{1}{2}} = \left[\frac{1}{2}\right]^{\frac{1}{2}} = \frac{1}{2}\sqrt{\pi},$$

where π is the half-circumference of the circle with radius 1 (1160).

Therefore, one obtains the simple equation for the differential equation of the curvature

$$y d^{\frac{1}{2}}v = v \sqrt{dy},$$

where dv is assumed to be constant. Utilizing the knowledge of the parameter $d^{\frac{1}{2}}v$, one transforms this equation to $\frac{y\sqrt{v}dv}{\frac{1}{2}\sqrt{\pi}} = v \sqrt{dy}$; And then both sides of the equation can be squared to obtain first $\frac{y^2 dv}{\frac{1}{4}\pi} = v dy$, and finally

$$\frac{1}{\frac{1}{4}\pi} 1v = C - \frac{1}{y}, \quad \text{ou} \quad y 1v = \frac{1}{4} C \pi y - \frac{1}{4} \pi.$$

Since this result is important not only in historical but also in mathematical sense, we clarify Lacroix reasoning using today's notation. Starting with the integer order n th derivative of the function $y(x) = x^m$, $m \in \mathbb{N}$ given by

$$\frac{d^n}{dx^n} y(x) = \frac{m!}{(m-n)!} x^{m-n}, \quad m \geq n,$$

Lacroix uses the generalized factorial, given by Euler's Gamma function, to formulate non-integer order derivatives and gets

$$\frac{d^n}{dx^n} y(x) = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}.$$

For the special case $y(x) = x$ and $n = 1/2$ Lacroix also presents the closed form representation

$$(1.1) \quad \frac{d^{1/2}}{dx^{1/2}} x = \frac{\Gamma(2)}{\Gamma(3/2)} x^{1/2} = \frac{2\sqrt{x}}{\sqrt{\pi}}.$$

The mathematical relevance of Lacroix work lies in the fact that his rather special result is the same as today's representation of the fractional derivative of Riemann-Liouville type (see equation (1.9) and Chapter 4.1.1).

Another more generally applicable definition of fractional operations was presented in the milestone book by J. B. J. Fourier [56] in 1822:

“We note that from equation (B) a very simple term for the differential coefficient of arbitrary order $\frac{d^i}{dx^i}fx$, as well as $\int^i dx^i \cdot fx$ can be derived. The sought-after term is a certain function of x and index i . [...] To gain this results, we remark that the expression $\cos \cdot (r + i\frac{\pi}{2})$, or

$$\cos \cdot r \cdot \cos \cdot \left(\frac{i\pi}{2}\right) - \sin \cdot r \cdot \sin \cdot \left(\frac{i\pi}{2}\right),$$

gradually becomes

$$- \sin \cdot r, - \cos \cdot r, + \sin \cdot r, + \cos \cdot r, - \sin \cdot r, \dots \text{etc.},$$

if the corresponding values of i are 1, 2, 3, 4, 5, etc. The same results recur in in the same series, if the value of i is increased Now one has to write in the second part of the equation

$$fx = \frac{1}{2\pi} \int d\alpha f\alpha \int dp \cos \cdot (px - p\alpha),$$

the factor p^i in front of the cosine and ad the term $+\frac{i\pi}{2}$ below the cosine. Thus one gets

$$\frac{d^i}{dx^i}fx = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\alpha f\alpha \int_{-\infty}^{+\infty} dp \cdot p^i \cdot \cos(px - p\alpha + i\frac{\pi}{2}).$$

The number i , which occurs in the second part, can be viewed as an arbitrary positive or negative quantity. [...]

The last equation using today's notation states

$$\frac{d^i}{dx^i}f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(\alpha)d\alpha \int_{-\infty}^{+\infty} p^i \cos \left(p(x - \alpha) + \frac{i\pi}{2} \right) dp,$$

where the number i which appears in the above will be regarded as any quantity whatsoever, positive or negative. This definition of a fractional derivative was the first one suitable for any sufficiently “well behaved” function (not necessarily a power function as in Lacroix’ paper, or the integral function in Laplace’s work).

With Fourier’s work we set the end of the early stages in the development of fractional calculus. What can be said about this stage is that almost from the beginning of classical calculus, the possibility of derivatives of fractional order were either discussed in letters, or being formulated in various ways. But it was not until 1823 that the first useful application of such derivatives became apparent, heralding the next stage of fractional calculus.

1.2 Abel’s integral equation and its impact on fractional calculus 1823-1916

Fractional calculus was mentioned from the beginning of classical calculus but it was not until 1823 before fractional operations were used to solve a specific physical problem. It

was Niels Henrik Abel who used this new mathematical tool to solve an integral equation arising in the *tautochrone problem* [1, 2]. The following excursus describes the problem and its solution in detail.

Excursus 1 (Tautochrone problem) *The tautochrone problem consists of the determination of a curve in the (x, y) plane such that the time required for a particle to slide down the curve to its lowest point under gravity is independent of its initial position (x_0, y_0) on the curve.*

The physical law states that the potential energy lost during the descent of the particle is equal to the kinetic energy the particle gains:

$$\frac{1}{2}m \left(\frac{d\lambda}{dt} \right)^2 = mg(y_0 - y),$$

where m is the mass of the particle, λ is the distance of the particle from the starting point along the curve and g is the gravitational acceleration. Separation of the time and space variables yields

$$-\frac{d\lambda}{\sqrt{y_0 - y}} = \sqrt{2g}dt$$

and integration from time $t = 0$ to time $t = T$ gives

$$\sqrt{2g}T = \int_0^{y_0} (y_0 - y)^{-1/2} d\lambda.$$

Given that the time the particle needs to reach the lowest point of the curve is supposed to be constant, the left hand side has to be a constant, say k . If we denote the path length λ as a function of height $\lambda = F(y)$ it follows that $d\lambda/dy = F'(y)$. By the change of variables $y_0 \rightarrow x$, $y \rightarrow t$ and denoting $F' = f$ the tautochrone integral equation becomes

$$(1.2) \quad k = \int_0^x (x - t)^{-1/2} f(t) dt,$$

where f is the function to be determined. By multiplying both sides of the integral equation with $1/\Gamma(1/2)$ Abel obtained on the right-hand side a fractional integral of order $1/2$:

$$\frac{k}{\Gamma(1/2)} = \frac{1}{\Gamma(1/2)} \int_0^x (x - t)^{-1/2} f(t) dt = \frac{d^{-1/2}}{dx^{-1/2}} f(x).$$

Utilizing the left-inverse of the fractional derivative, i.e.

$$\frac{d^{1/2}}{dx^{1/2}} \frac{d^{-1/2}}{dx^{-1/2}} f(x) = \frac{d^0}{dx^0} f(x) = f(x)$$

the solution of the tautochrone problem is then given by

$$f(x) = \frac{1}{\Gamma(1/2)} \frac{d^{1/2}}{dx^{1/2}} k = \frac{k}{\pi \sqrt{x}},$$

where for the last equality the derivative of order $1/2$ of a constant k has been used.

As Samko et al. pointed out in their book [141] it is important to note that Abel not only solved the integral equation (1.2) as the special case of the tautochrone problem, but instead gave the solution for the more general integral equation

$$k(x) = \int_a^x \frac{f(t)}{(x-t)^\alpha} dt, \quad x > a, \quad 0 < \alpha < 1.$$

After Abel's application of fractional operators to a problem in physics the first broad study of fractional calculus were carried out in a series of papers [84]-[91] by J. Liouville. In [86] Liouville developed two different definitions of fractional derivatives. The first is applied on functions $f(x)$ which can be expanded in a series of the following form

$$f(x) = \sum_{k=0}^{\infty} c_k \exp(a_k x).$$

By extending the known integer order derivatives $d^n/dx^n \exp(ax) = D^n e^{ax} = a^n e^{ax}$ to the fractional case (formally replacing $n \in \mathbb{N}$ with $\alpha \in \mathbb{C}$) he obtained

$$(1.3) \quad D^\alpha f(x) = \sum_{k=0}^{\infty} c_k a_k^\alpha \exp(a_k x).$$

This definition is obviously restricted to choices of α for which the series (1.3) converges. The second definition developed in [86] does not have such a restriction on the choice of α , but instead has a stronger restriction on the type of function for which it is applicable: For functions of the type $f(x) = 1/x^a$, with an arbitrary parameter a , Liouville developed the definition

$$(1.4) \quad D^\alpha x^{-a} = \frac{(-1)^\alpha \Gamma(a + \alpha)}{\Gamma(a)} x^{-a-\alpha}$$

for its fractional derivative of order α . Even though both definitions given in [86] are restricted in their own way, Liouville used these definitions in later parts of his paper [86] for a number of applications to geometrical, physical and mechanical problems.

The eight papers [84]-[91] by Liouville contain a large number of theoretical and applied results and it would go beyond the scope of this work to give an overview of them all. But two aspects are of particular importance for historical reasons: As Samko et al. discussed in their book [141], Liouville considered in [86] the use of differences of fractional order to define fractional derivatives as a limit of a difference quotient. While Liouville did not develop this idea in greater detail, it will return at a later time in history as the Grünwald-Letnikov definition of fractional derivatives (see equation (1.10) and Chapter 4.1.3). The second historical noteworthy aspect concerns the so called *complementary function*. Liouville states in [87] that the ordinary differential equation $d^n y/dx^n = 0$ has the complementary solution $y_c = c_0 + c_1 x + c_2 x^2 + \dots + c_{n-1} x^{n-1}$ (which defines the band of solutions if no initial conditions are defined) and states that a similar complementary function y_c should exist for the differential equation $d^\alpha y/dx^\alpha = 0$ of arbitrary order α . This statement is important for at least two reasons: On the one hand at the time Liouville stated the existence of such a complementary function a number of definitions of fractional derivatives were already existing (Lacroix', Laplace's, Fourier's, Abel's and Liouville's). Those different definitions

lead to different complementary functions - contrary to the integer case - and this undetermined status of *one* complementary function was the origin of “a longstanding controversy” (see [135]) in this new mathematical field, which decimated the trust in the general theory of fractional operations in its youth. On the other hand complementary functions are used by Riemann for his definition of fractional derivatives as we will see next and thus had an impact on the historical development of fractional calculus.

In 1847 G. F. B. Riemann worked on a paper where, searching for a generalization of a Taylor series, he deduced the definition

$$(1.5) \quad D^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x-t)^{\alpha-1} f(t) dt + \psi(x)$$

for a fractional integral of order α of a given function $f(x)$. The function $\psi(x)$ is introduced because of the ambiguity of the lower limit c of integration and as such corresponds to the complementary function mentioned in the work by Liouville. Equation (1.5) with lower limit $c = 0$ and without a complementary function $\psi(x)$ is (together with the reasoning by Liouville - equation (1.3)) the most common definition of fractional integration today, called *Riemann-Liouville fractional integral* (see also Chapter 4.1.1). However, Riemann himself did not deduce rigorously the representation without the problematic complementary function, which is not a triviality, as A. Cayley pointed out in [23]: “The greatest difficulty [...] is the question of the meaning of a complementary function containing an infinity of arbitrary constants”. It is also historically notable that Riemann did not publish this work himself; it was posthumously printed in his collected works [148] ten years after his death.

Since neither Riemann nor Liouville solved the problem of the complementary function it is of historical interest how today’s Riemann-Liouville definition was finally deduced. A number of people are responsible for this development: In 1869 N. Y. Sonin [142] wrote a paper, where he used Cauchy’s Integral formula as a starting point to reach differentiation with arbitrary index. A. V. Letnikov extended the idea of Sonin a short time later in 1872 in his paper [82]. Both tried to define fractional derivatives by utilizing a closed contour. Starting with Cauchy’s integral formula for integer order derivatives, given by

$$(1.6) \quad f^{(n)}(z) = \frac{n!}{2\pi i} \int_C \frac{f(t)}{(t-z)^{n+1}} dt,$$

the generalization to the fractional case can be obtained by replacing the factorial with Euler’s Gamma function $\alpha! = \Gamma(\alpha + 1)$ (see Chapter 3.2 for a formal definition). However, the direct extension to non-integer values α results in the problem that the integrand in (1.6) contains a branch point, and as Ross points out in [135] “An appropriate contour would then require a branch cut which was not included in the work of Sonin and Letnikov”. In the end it was the work of H. Laurent [79], who used a contour given as an open circuit (today known as *Laurent loop*) instead of a closed circuit used by Sonin and Letnikov and thus produced today’s definition of the *Riemann-Liouville fractional integral*:

$$(1.7) \quad {}_c D_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x-t)^{\alpha-1} f(t) dt, \quad \operatorname{Re}(\alpha) > 0$$

by standard contour integration methods. A number of remarks need to be made with respect to the definition given in equation (1.7): The notation ${}_c D_x^{-\alpha} f(x)$, which is still used in

some modern textbooks for the fractional integral (and by replacing $-\alpha$ with α in the notation for the fractional derivative) was first introduced by H. T. Davis in [30] and is thus not the notation used in the cited papers. But in a way it is a minimized representation dealing with the different parameters of fractional integrals and derivatives, namely the order α , the variable x and the lower index of integration. The lower index is of particular importance; By choosing $c = 0$ in (1.7) one gets Riemann's formula (1.5) without the problematic complementary function $\psi(x)$ and by choosing $c = -\infty$, formula (1.7) is equivalent to Liouville's first definition (1.3). These two facts explain why equation (1.7) is called Riemann-Liouville fractional integral.

While the notation of fractional integration and differentiation only differ in the sign of the parameter α in (1.7), the change from fractional integration to differentiation cannot be achieved directly by replacing the sign of α on the right-hand side of (1.7). The problem originates from the integral $\int_c^x (x-t)^{-\alpha-1} f(t) dt$, which is divergent in general. However, by analytic continuation it can be shown that

$$(1.8) \quad {}_c D_x^\alpha f(x) = {}_c D_x^{n-\beta} f(x) = {}_c D_{x,c}^n D_x^{-\beta} f(x) = \frac{d^n}{dx^n} \left(\frac{1}{\Gamma(\beta)} \int_c^x (x-t)^{\beta-1} f(t) dt \right)$$

holds, which is known today as the definition of the *Riemann-Liouville fractional derivative*. In (1.8) $n = \lceil \alpha \rceil$ is the smallest integer greater than α and $0 < \beta = n - \alpha < 1$. For either $c = 0$ or $c = \infty$ the integral in (1.8) is the beta integral (see e.g. Theorem 3.3.1) for a wide class of functions and thus easily evaluated. Using the definition (1.8) it can easily be shown that Riemann's fractional derivative ($c = 0$) for a function $f(x) = x^a$ with an arbitrary parameter a is given by

$$(1.9) \quad {}_0 D_x^\alpha x^a = \frac{\Gamma(a+1)}{\Gamma(a-\alpha+1)} x^{a-\alpha},$$

which for $a = 1/2$ coincides with the early example (1.1) produced by Lacroix.

Nearly simultaneously to the paper by Sonin [142], starting the mathematical basis for today's version of the Riemann-Liouville fractional integral, two papers, one by Grünwald [62] and one by Letnikov [81] provided the basis for another definition of fractional derivatives which is also frequently used today. Carrying out the mathematics behind the earlier mentioned idea of Liouville, to use the limit of a difference quotient using differences of fractional order, Grünwald and Letnikov obtained

$$(1.10) \quad {}^{GL} D_x^\alpha f(x) = \lim_{h \rightarrow 0} \frac{(\Delta_h^\alpha f)(x)}{h^\alpha}$$

as definition of fractional differentiation, which today is called *Grünwald-Letnikov fractional derivative*. In definition (1.10) the finite differences Δ_h^α are defined as

$$(\Delta_h^\alpha f)(x) = \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x - kh), \quad \alpha > 0$$

and $\binom{\alpha}{k}$ is the generalized binomial coefficient, wherein the factorials are replaced with Euler's Gamma function (see further Chapter 4.1.3). An important result in the paper by

Letnikov [81] is that the Grünwald-Letnikov definition coincides under certain conditions with the definitions given by Riemann and Liouville. The Grünwald-Letnikov definition of fractional derivatives is today mainly used for numerical methods, which use formula (1.10) with a finite sum to approximate fractional derivatives (see Chapter 5.1.1).

Together with the advances in fractional calculus at the end of the nineteenth century the work of O. Heaviside [69] has to be mentioned. Today his work is collected under the name *Heaviside operational calculus* and is based on the idea that the differential operator d/dx is replaced by a letter p and treated as a constant in the solution of differential equations. The connection to fractional calculus is established by the fact that Heaviside used arbitrary powers of p , mostly $p^{1/2}$, to obtain solutions in engineering problems. As Ross pointed out in [135] “He (Heaviside) interpreted $p^{1/2} \rightarrow 1$, that is, $D^{1/2}1$ to mean $1/(\pi t)^{1/2}$ ”, and since $f(x) = 1$ is a function of the Riemann class, Heaviside’s operator can be interpreted as Riemann operator ${}_0D_x^\alpha$ and thus shows another early application of fractional calculus.

At this point in time we set another stop in the history of fractional calculus. In this nearly century long period fractional operations were applied to scientific problems outside pure mathematics starting with Abel’s tautochrone problem. In addition the first detailed work on the theory of fractional calculus started with the papers of Liouville and was followed by the work of several other mathematicians. In the first two sections we could go into most letters, papers and books concerned with fractional calculus. The next time period cannot be considered with the same level of detail due to the fact that by the beginning of the twentieth century fractional calculus had already grown to a broad mathematical field of its own.

1.3 From Riesz and Weyl to modern fractional calculus (1917 to present)

The Riemann-Liouville definition of a fractional integral given in (1.7) with lower limit $c = -\infty$ is often referred to as *Weyl fractional integral*. The reason for this lies in a paper of H. Weyl [151] published 1917. In this paper Weyl considered the Fourier transform of periodic functions $\varphi(x)$, given by

$$\sum_{k=-\infty}^{\infty} \varphi_k e^{ikx}, \quad \varphi_k = \frac{1}{2\pi} \int_0^{2\pi} e^{ikx} \varphi(x) dx$$

in order to define fractional integration suitable for these functions, by

$$(1.11) \quad I_{\pm}^{\alpha} \varphi(x) = \frac{1}{2\pi} \int_0^{2\pi} \Psi_{\pm}^{\alpha}(x-t) \varphi(t) dt,$$

with some special functions $\Psi_{\pm}^{\alpha}(x)$. Moreover, he showed that these fractional integrals can be written for $0 < \alpha < 1$ as

$$(1.12) \quad I_{+}^{\alpha} \varphi(x) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^x (x-t)^{\alpha-1} \varphi(t) dt, \quad I_{-}^{\alpha} \varphi(x) = \frac{1}{\Gamma(\alpha)} \int_x^{\infty} (x-t)^{\alpha-1} \varphi(t) dt$$

given that the integrals in (1.12) are convergent over an infinite interval. In Weyl's paper this convergence is guaranteed by considering only those periodic functions $\varphi(x)$, whose Fourier transform fulfill $\varphi_0 = 0$. This is an important fact, as noted by Samko et al. in [141], since today's definitions of Weyl integrals usually do not mention this detail. Since the Riemann-Liouville definition (1.7) already considered integration over an infinite interval, naming equation (1.12) as Weyl's integral is historically incorrect. In [151] Weyl also showed that a periodic function $\varphi(x)$ has a continuous derivative of order α if it fulfills a Lipschitz condition of order $\lambda > \alpha$.

In 1927 Marchaud [103] developed an integral version of the Grünwald-Letnikov definition (1.10) of fractional derivatives, using

$$(1.13) \quad {}^M D^\alpha f(x) = c \int_0^\infty \frac{(\Delta_t^\ell f)(x)}{t^{1+\alpha}} dt, \quad \alpha > 0,$$

as fractional derivative of a given function f , today known as *Marchaud fractional derivative*. The term $(\Delta_t^\ell f)(x)$ is a finite difference of order $\ell > \alpha$ and c is a normalizing constant. Definition (1.13) coincides under certain conditions with the Riemann-Liouville and Grünwald-Letnikov version of fractional derivatives.

Concerning mapping properties of fractional integration the work of Hardy and Littlewood [67] needs to be mentioned. In [67] they proved that a fractional integration operator of order α maps a function of L_p into L_q , where $q^{-1} = p^{-1} - \alpha$. In a subsequent paper [68] they developed additional mapping properties in Lipschitzian spaces, which influenced not only fractional calculus, but functional analysis and function theory as well.

In 1931 Watanabe [147] developed a Leibniz' formula for Riemann-Liouville's fractional derivative, given by

$$(1.14) \quad D^\alpha(fg) = \sum_{k=-\infty}^{\infty} \binom{\alpha}{k+\beta} D^{\alpha-\beta-k} f D^{\beta+k} g, \quad \beta \in \mathbb{R}$$

for analytic functions f and g .

M. Riesz started 1938 to published a number of papers [128, 129] (more detailed in later papers [130, 131]) which are centered around the integral

$$(1.15) \quad {}^R I^\alpha \varphi = \frac{1}{2\Gamma(\alpha) \cos(\alpha\pi/2)} \int_{-\infty}^{\infty} \frac{\varphi(t)}{|t-x|^{1-\alpha}} dt, \quad \operatorname{Re} \alpha > 0, \quad \alpha \neq 1, 3, 5, \dots$$

today known as *Riesz potential*. This integral (and its generalization in the n -dimensional Euclidean space, which is also regarded in [128, 129]) is tightly connected to Weyl fractional integrals (1.12) and therefore to the Riemann-Liouville fractional integrals by

$${}^R I^\alpha = (I_+^\alpha + I_-^\alpha)(2 \cos(\alpha\pi/2))^{-1}.$$

A paper by B. S. Nagy [108] contributed to the field of approximation theory. He developed a Favard type inequality for trigonometric sums $f(y) = \sum_{|k| \geq m} f_k e^{ikx}$

$$\|I_\pm^\alpha f\|_{L_\infty} \leq \frac{c}{m^\alpha} \|f\|_{L_\infty},$$

with some constant c . He also obtained a Bernstein-type theorem on the rate of approximation of fractional integrals by trigonometric polynomials. Those results had important impact on the theory of approximation by trigonometric polynomials, as pointed out by Samko et al. in [141].

A modification of the Riemann-Liouville definition of fractional integrals, given by

$$(1.16) \quad \frac{2x^{-2(\alpha+\eta)}}{\Gamma(\alpha)} \int_0^x (x^2 - t^2)^{\alpha-1} t^{2\eta+1} \varphi(t) dt, \quad \frac{2x^{2\eta}}{\Gamma(\alpha)} \int_0^\infty (t^2 - x^2)^{\alpha-1} t^{1-2\alpha-2\eta} \varphi(t) dt$$

were introduced by Erdélyi and Kober in [47, 48], which became useful in various applications. While these ideas are tightly connected to fractional differentiation of the functions x^2 and \sqrt{x} , already done by Liouville 1832 in [86], the fact that Erdélyi and Kober used the Mellin transform for their results is noteworthy.

A great number of additional results of fractional calculus were presented in the twentieth century, but at this point we only concentrate on one more, given by M. Caputo and first used extensively in [20]. Given a function f with an $(n-1)$ absolute continuous derivative, Caputo defined a fractional derivative by

$$(1.17) \quad D_*^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{n-\alpha-1} \left(\frac{d}{ds} \right)^n f(s) ds$$

today usually named *Caputo fractional derivative*. The derivative (1.17) is strongly connected to the Riemann-Liouville fractional derivative (see Chapter 4.1.2) and is today frequently used in applications. This is because using the Caputo derivative one can specify the initial conditions of fractional differential equations in classical form, i.e.

$$y^{(k)}(0) = b_k, \quad k = 0, 1, \dots, n-1,$$

in contrast to differential equations containing the Riemann-Liouville differential operator (see Chapter 4.2). While the operator D_*^α is denoted today as Caputo operator, Y. N. Rabotnov had already introduced this differential operator into the Russian viscoelastic literature in [125], a year before Caputo's paper was published.

By the second half of the twentieth century the field of fractional calculus had grown to such extent, that in 1974 the first conference concerned solely with the theory and applications of fractional calculus was held in New Haven [134]. In the same year the first book on fractional calculus by Oldham and Spanier [110] was published. A number of additional books have appeared since then, the most popular the ones by Miller and Ross [105] (1993), Samko et al. [141] (1993) and Podlubny [122] (1999). In 1998 the first issue of the mathematical journal "Fractional calculus & applied analysis" was printed. This journal is solely concerned with topics on the theory of fractional calculus and its applications. Finally in 2004 the large conference "Fractional differentiation and its applications" was held in Bordeaux, where no less than 104 talks were given in the field of fractional calculus.

From its birth - a simple question from L'Hospital to Leibniz - to its today's wide use in numerous scientific fields *fractional calculus* has come a long way. Even though its nearly as old as classical calculus itself, it flourished mainly over the last decades because of its good applicability on models describing complex real life problems (see Chapter 6 for some examples). And even though the term *fractional calculus* is a misnomer we will use it throughout this text, which will be concerned with theoretical and, more importantly, numerical aspects of problems arising in this field.

Chapter 2

Integer calculus

Integer (or classical) calculus is a well researched mathematical field and results can be found in numerous books on analysis, differentiation and integration, differential equations, integral equations, partial differential equations etc. While only integer order derivatives and integrals are addressed in this mathematical field, the results can often be carried over to the fractional case. For this reason important results of integer calculus are outlined in this chapter. We consider both analytical and numerical aspects of classical calculus for their use in the upcoming corresponding chapters on fractional calculus. Since all of the stated results are well known, the proofs are omitted.

2.1 Integration and differentiation

Integer order integration and differentiation is tightly connected by the well known fundamental theorem of classical calculus [138, Thm. 6.18]:

Theorem 2.1.1 (Fundamental Theorem of Classical Calculus) *Let $f : [a, b] \rightarrow \mathbb{R}$ be a continuous function and let $F : [a, b] \rightarrow \mathbb{R}$ be defined by*

$$F(x) = \int_a^x f(t)dt.$$

Then, F is differentiable and

$$F'(x) = f(x).$$

One important goal of fractional calculus is to retain this relation in a generalized sense. Before we go back to this goal in Chapter 4, it is fruitful to state some additional results of classical calculus. To keep a consistent notation throughout this thesis (in the integer as well as the fractional case), we will use the following notations from now on:

Definition 2.1.1 1. *By D we denote the operator that maps a differentiable function onto its derivative, i.e.*

$$Df(x) := f'(x) = \frac{d}{dx}f(x).$$

2. By J_a , we denote the operator that maps a function f , assumed to be (Riemann) integrable on the compact interval $[a, b]$, onto its primitive centered at a , i.e.

$$J_a f(x) := \int_a^x f(t) dt$$

for $a \leq x \leq b$. If $a = 0$ we will simply write J instead of J_0 .

3. For $n \in \mathbb{N}$ we use the symbols D^n and J_a^n to denote the n -fold iterates of D and J_a , respectively, i.e. we set $D^1 := D$, $J_a^1 := J_a$, and $D^n := DD^{n-1}$ and $J_a^n := J_a J_a^{n-1}$ for $n \geq 2$.

A first result, which will be most important for the later generalization to non-integer integrals, can be obtained from this definition. Utilizing the recursive formula of part three in Definition 2.1.1 we can give an explicit formula of the integral operator J_a^n , $n \in \mathbb{N}$:

Lemma 2.1.2 *Let f be Riemann integrable on $[a, b]$. Then, for $a \leq x \leq b$ and $n \in \mathbb{N}$, we have*

$$J_a^n f(x) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt.$$

From this Lemma another consequence can be drawn. In terms of Definition 2.1.1 the fundamental theorem of classical calculus reads $DJ_a f = f$, which implies by Definition 2.1.1 3. that $D^n J_a^n f = f$. This leads to the following Lemma:

Lemma 2.1.3 *Let $m, n \in \mathbb{N}$ such that $m > n$, and let f be a function having a continuous n th derivative on the interval $[a, b]$. Then,*

$$D^n f = D^m J_a^{m-n} f.$$

Before stating additional properties of integral and differential operators it is necessary to introduce some classical function spaces, in which the upcoming results will be formulated.

Definition 2.1.2 *Let $0 < \mu \leq 1$, $k \in \mathbb{N}$ and $1 \leq p$. We define:*

$$L_p[a, b] := \left\{ f : [a, b] \rightarrow \mathbb{R}; f \text{ is measurable on } [a, b] \right.$$

$$\left. \text{and } \int_a^b |f(x)|^p dx < \infty \right\},$$

$$L_\infty[a, b] := \{ f : [a, b] \rightarrow \mathbb{R}; f \text{ is measurable and essentially bounded on } [a, b] \},$$

$$H_\mu[a, b] := \{ f : [a, b] \rightarrow \mathbb{R}; \exists c > 0 \forall x, y \in [a, b] : |f(x) - f(y)| \leq c|x - y|^\mu \},$$

$$C^k[a, b] := \{ f : [a, b] \rightarrow \mathbb{R}; f \text{ has a continuous } k\text{th derivative} \},$$

$$C[a, b] := C^0[a, b],$$

$$H_0[a, b] := C[a, b].$$

For $1 \leq p \leq \infty$ the function space $L_p[a, b]$ is the usual *Lebesgue space*, whereas $H_\mu[a, b]$ is a *Lipschitz* or *Hölder space* of order μ . For later use we state a formulation of the Fundamental Theorem 2.1.1 in the Lebesgue space:

Theorem 2.1.4 (Fundamental Theorem in Lebesgue Space) *Let $f \in L_1[a, b]$. Then, $\int_a f$ is differentiable almost everywhere in $[a, b]$, and $D\int_a f = f$ also holds almost everywhere on $[a, b]$.*

A number of rules for operations on functions and their derivatives is known in classical calculus: The product rule, the quotient rule and the chain rule give each a simple representation for the derivatives of the multiplication, division and concatenation of two continuously differentiable functions. In more detail those rules are given by:

Theorem 2.1.5 (Product rule) *Let $f, g \in C[a, b]$. Then,*

$$D(fg)(x) = Df(x)g(x) + f(x)Dg(x).$$

Theorem 2.1.6 (Quotient rule) *Let $f, g \in C[a, b]$ and $g(x) \neq 0$. Then,*

$$D\frac{f}{g}(x) = \frac{Df(x)g(x) - f(x)Dg(x)}{g(x)^2}.$$

Theorem 2.1.7 (Chain rule) *Let $f, g \in C[a, b]$. Then,*

$$Dg(f(x)) = \frac{d}{df(x)}g(f(x))Df(x).$$

Repeated use of the product rule gives the following well known Leibniz' formula, which can easily be proven by induction:

Theorem 2.1.8 (Leibniz' formula) *Let $n \in \mathbb{N}$, and let $f, g \in C^n[a, b]$. Then,*

$$D^n[fg] = \sum_{k=0}^n \binom{n}{k} (D^k f)(D^{n-k} g).$$

There also exists a generalization of the chain rule, which, however, is not commonly used. But since we will need it for a numerical method later on, we will state it here and give an example.

Theorem 2.1.9 (Faà di Bruno's formula - set partition version) *Let $n \in \mathbb{N}$, and f and g be functions with a sufficient number of derivatives. Then*

$$D^n g(f(x)) = \sum g^{(k)}(f(x)) (f'(x))^{b_1} (f''(x))^{b_2} \dots (f^{(n)}(x))^{b_n}$$

where the sum is over all partitions of $\{1, 2, \dots, n\}$ and for each partition, k is its number of blocks and b_i is the number of blocks with exactly i elements.

Example 2.1.1 *Let us consider the fourth derivative of the function $g(f(x))$. We need to find all partitions of $\{1, 2, 3, 4\}$ and count their blocks and the elements in each block. We thus get:*

Partitions	Blocks / elements and resulting values for b_i
$\{1, 2, 3, 4\}$	1 block with 4 elements $\rightarrow b_4 = 1$
$\{1\}, \{2, 3, 4\}$	2 blocks with 1 and 3 elements respectively $\rightarrow b_1 = 1, b_3 = 1$
$\{2\}, \{1, 3, 4\}$	2 blocks with 1 and 3 elements respectively $\rightarrow b_1 = 1, b_3 = 1$
$\{3\}, \{1, 2, 4\}$	2 blocks with 1 and 3 elements respectively $\rightarrow b_1 = 1, b_3 = 1$
$\{4\}, \{1, 2, 3\}$	2 blocks with 1 and 3 elements respectively $\rightarrow b_1 = 1, b_3 = 1$
$\{1, 2\}, \{3, 4\}$	2 blocks with 2 elements each $\rightarrow b_2 = 2$
$\{1, 3\}, \{2, 4\}$	2 blocks with 2 elements each $\rightarrow b_2 = 2$
$\{1, 4\}, \{2, 3\}$	2 blocks with 2 elements each $\rightarrow b_2 = 2$
$\{1\}, \{2\}, \{3, 4\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{1\}, \{3\}, \{2, 4\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{1\}, \{4\}, \{2, 3\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{2\}, \{3\}, \{1, 4\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{2\}, \{4\}, \{1, 3\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{3\}, \{4\}, \{1, 2\}$	3 blocks with 1, 1 and 2 elements respectively $\rightarrow b_1 = 2, b_2 = 1$
$\{1\}, \{2\}, \{3\}, \{4\}$	4 blocks with 1 element each $\rightarrow b_1 = 4$

Taking the sum over all partitions we thus get:

$$D^4 g(f(x)) = g'(f(x))f^{(4)}(x) + 4g''(f(x))f'(x)f'''(x) + 3g''(f(x))[f''(x)]^2 + 6g'''(f(x))[f'(x)]^2 f''(x) + g^{(4)}(f(x))[f'(x)]^4.$$

This formula is obviously not as elegant as the other ones. Nevertheless it states an important result on the general structure of the n th derivative of a concatenated function, which we will need in the Chapter 5.2 on Adomian's Decomposition method.

Another result, which is used quite often in classical calculus, is Taylor's Theorem. Instead of using the classical formulation we give a more instructive definition. But before we can do that, we need to introduce another function space:

Definition 2.1.3 By A^n or $A^n[a, b]$ we denote the set of functions with an absolutely continuous $(n-1)$ st derivative, i.e. the functions f for which there exists (almost everywhere) a function $g \in L_1[a, b]$ such that

$$f^{(n-1)}(x) = f^{(n-1)}(a) + \int_a^x g(t)dt.$$

In this case we call g the (generalized) n th derivative of f , and we simply write $g = f^{(n)}$.

Theorem 2.1.10 (Taylor expansion) For $m \in \mathbb{N}$ the following statements are equivalent:

1. $f \in A^m[a, b]$.
2. For every $x, y \in [a, b]$,

$$f(x) = \sum_{k=0}^{m-1} \frac{(x-y)^k}{k!} D^k f(y) + J_y^m D^m f(x).$$

To obtain the classical form of Taylor's Theorem from Theorem 2.1.10 one needs to choose $y = a$ and use only the implication $(a) \Rightarrow (b)$ instead of the equivalence. If $y = 0$ the expansion is also known as the *Maclaurin series*. An important part of the Taylor expansion is its polynomial:

Definition 2.1.4 Let $f(x) \in C^n[a, b]$ and $x_0 \in [a, b]$. The polynomial

$$T_n[f, x_0](x) = \sum_{k=0}^n \frac{(x - x_0)^k}{k!} D^k f(x_0)$$

is called the Taylor polynomial of order n , centered at x_0 .

For some proofs in later chapters we will need information under which circumstances the order of integration of a double integral can be interchanged:

Theorem 2.1.11 (Fubini's Theorem) Let $[a, b]$ and $[c, d]$ be two compact intervals, f be a Riemann-integrable function and assume that

$$g(y) = \int_a^b f(x, y) dx \quad \text{exists for every fixed } y \in [c, d].$$

Then, g is Riemann-integrable on $[c, d]$ and

$$(2.1) \quad \int_{[a,b] \times [c,d]} f(x, y) d(x, y) = \int_c^d \left(\int_a^b f(x, y) dx \right) dy.$$

If furthermore

$$h(y) = \int_c^d f(x, y) dy \quad \text{exists for every fixed } x \in [a, b]$$

then

$$(2.2) \quad \int_a^b \left(\int_c^d f(x, y) dy \right) dx = \int_c^d \left(\int_a^b f(x, y) dx \right) dy = \int_{[a,b] \times [c,d]} f(x, y) d(x, y).$$

We have addressed most of the analytical results on integer order differentiation and integration, which we will either need in later chapters on fractional calculus or restate in the fractional setting. However, for some proofs in the upcoming sections and chapters several fixed point theorems are needed, so we state them in this section even though they are not results in the field of integration and differentiation in a strict sense. We start with Weissinger's fixed point theorem that we take from [149]:

Theorem 2.1.12 (Weissinger's Fixed Point Theorem) Assume (U, d) to be a nonempty complete metric space, and let $\alpha_j \geq 0$ for every $j \in \mathbb{N}_0$ and such that $\sum_{j=0}^{\infty} \alpha_j$ converges. Moreover, let the mapping $A : U \rightarrow U$ satisfy the inequality

$$(2.3) \quad d(A^j u, A^j v) \leq \alpha_j d(u, v)$$

for every $j \in \mathbb{N}$ and every $u, v \in U$. Then, A has a uniquely defined fixed point u^* . Furthermore, for any $u_0 \in U$, the sequence $(A^j u_0)_{j=1}^{\infty}$ converges to this fixed point u^* .

An immediate consequence of Weissinger's theorem, is the one usually connected with the name of Banach:

Corollary 2.1.13 (Banach's Fixed Point Theorem) *Assume (U, d) to be a nonempty complete metric space, let $0 \leq \alpha < 1$, and let the mapping $A : U \rightarrow U$ satisfy the inequality*

$$(2.4) \quad d(Au, Av) \leq \alpha d(u, v)$$

for every $u, v \in U$. Then, A has a uniquely defined fixed point u^ . Furthermore, for any $u_0 \in U$, the sequence $(A^j u_0)_{j=1}^\infty$ converges to this fixed point u^* .*

Moreover, we will need a slightly different result that asserts only the existence but not the uniqueness of a fixed point in later sections of this text. A weaker assumption on the operator in question leads to Schauder's theorem. A proof may be found, e.g., in [25].

Theorem 2.1.14 (Schauder's Fixed Point Theorem) *Let (E, d) be a complete metric space, let U be a closed convex subset of E , and let $A : U \rightarrow U$ be a mapping such that the set $\{Au : u \in U\}$ is relatively compact in E . Then A has got at least one fixed point.*

In this context we recall a definition:

Definition 2.1.5 *Let (E, d) be a metric space and $F \subseteq E$. The set F is called relatively compact in E if the closure of F is a compact subset of E .*

Another helpful result from Analysis in connection with these sets is the following.

Theorem 2.1.15 (Arzelà-Ascoli) *Let $F \subseteq C[a, b]$ for some $a < b$, and assume the sets to be equipped with the Chebyshev norm. Then, F is relatively compact in $C[a, b]$ if and only if F is equicontinuous (i.e. for every $\varepsilon > 0$ there exists some $\delta > 0$ such that for all $f \in F$ and all $x, x^* \in [a, b]$ with $|x - x^*| < \delta$ we have $|f(x) - f(x^*)| < \varepsilon$) and uniformly bounded (i.e. there exists a constant $C > 0$ such that $\|f\|_\infty \leq C$ for every $f \in F$).*

Having established basic results on integer order integration and differentiation and also stated some fixed point theorems, we consider results on ordinary differential equations in the next section and explain a class of numerical methods frequently used to solve them.

2.2 Differential equations and multistep methods

In this section we give a brief overview of the theory of ordinary differential equations and in addition explain the idea of multistep methods. Our goal is not to construct an exhaustive mathematical structure, but rather to pick some important results which we will try to formulate in later chapters for the fractional case. Therefore in some parts we will not proceed in the usual fashion used for an introduction in ordinary differential equations. We start this section with a formal definition of an ordinary differential equation.

Definition 2.2.1 Let $n \in \mathbb{N}$ and $f : A \subseteq \mathbb{R}^2 \rightarrow \mathbb{R}$. Then

$$(2.5) \quad D^n y(x) = f(x, y(x))$$

is called ordinary differential equation of order n . If additionally initial conditions of the form

$$(2.6) \quad D^k y(0) = b_k \quad (k = 0, 1, \dots, n-1)$$

are defined we understand the differential equation (2.5), equipped with initial conditions (2.6) as initial value problem.

Usually a more general definition is used, which admits the possibility of *multiterm* and *implicit* ordinary differential equations, i.e. equations of the form

$$F(x, y(x), Dy(x), D^2y(x), \dots, D^n y(x)) = 0, \quad F : A \subseteq \mathbb{R}^{n+2} \rightarrow \mathbb{R}$$

instead of the one given in (2.5). Furthermore, the initial conditions usually are defined at an initial point x_0 instead of 0 as in (2.6). But, as mentioned above, we restrict ourself in this chapter on simple cases of ordinary differential equations, and thus use Definition 2.2.1.

A first result, which will become fundamental for the fractional case is the equivalence of an ordinary differential equation to an integral equation, given in the following lemma:

Lemma 2.2.1 The function $y(x)$ is a solution to the differential equation (2.5) equipped with initial condition (2.6) if and only if $y(x)$ is a solution of the integral equation

$$(2.7) \quad y(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} D^k y(0) + \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t, y(t)) dt$$

Proof: The proof of this lemma is easily obtained; One only needs to apply the classical differential or integral operator in connection with Lemma 2.1.2 to obtain both directions of the proof. \square

The question of existence and uniqueness of a solution of an ordinary differential equation (2.5) equipped with initial conditions (2.6) is answered by the classical theorems of Peano and Picard-Lindelöf:

Theorem 2.2.2 (Peano's Existence Theorem) Let $c > 0$ and $G := \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq 0 + c\}$ and $f : G \rightarrow \mathbb{R}$. be continuous. Then the ordinary differential equation (2.5) equipped with initial conditions (2.6) possesses at least one solution in a neighborhood $U \subseteq [0, 0 + c]$.

Theorem 2.2.3 (Picard-Lindelöf's Existence and Uniqueness Theorem) Let $c > 0$ and $G := [0, 0 + c] \times \mathbb{R}$ and assume that the function $f : G \rightarrow \mathbb{R}$ is continuous and that it fulfills a Lipschitz condition with respect to the second variable, i.e. there exists a constant $L > 0$ such that, for all (x, y_1) and $(x, y_2) \in G$, we have

$$|f(x, y_1) - f(x, y_2)| < L|y_1 - y_2|.$$

Then the ordinary differential equation (2.5) equipped with initial conditions (2.6) possesses a uniquely defined solution.

Besides the existence and uniqueness of a solution for an ordinary differential equation (2.5), results on the behavior of the solution derived only from the knowledge of the function f are important. Before we state some results in this direction we need to introduce another definition:

Definition 2.2.2 Let $n \in \mathbb{N}$, $G \subseteq \mathbb{R}^n$ and $f \in C(G)$. Then the function f is called analytic in G , if for any point $(v_1, v_2, \dots, v_n) \in G$ there exists a power series satisfying

$$f(x_1, x_2, \dots, x_n) = \sum_{\mu_1, \dots, \mu_n=0}^{\infty} c_{\mu_1, \dots, \mu_n} (x - v_1)^{\mu_1} (x - v_2)^{\mu_2} \dots (x - v_n)^{\mu_n},$$

which is absolutely convergent in a neighbourhood of (v_1, v_2, \dots, v_n) .

A first result on the properties of the solution of an ordinary differential equation (2.5) states under which conditions an analytic solution is ensured:

Theorem 2.2.4 If the function f of the differential equation (2.5) equipped with initial conditions (2.6) is analytic in a neighbourhood of $(0, Dy(0), \dots, D^n y(0))$, the solution of (2.5) is analytic in a neighbourhood of 0.

The question of differentiability of the solution can also be assured for ordinary differential equations:

Theorem 2.2.5 Let $k \in \mathbb{N}$, $b > 0$ and $f \in C^k([0, b] \times \mathbb{R})$. Then the solution of the initial value problem

$$Dy(x) = f(x, y(x)), \quad y(0) = b_0$$

is $(k + 1)$ -times differentiable.

In the following part of this section we are interested in a numerical method for solving a first order differential equation with a given initial condition. This means we are interested in a solution y on a closed interval $[0, X]$ for some $X > 0$. In general numerical methods do not produce a solution on the whole interval in question, but rather give the solution on a prescribed set of nodes in the interval. Therefore we assume from now on that the nodes are arranged equispaced inside the interval $[0, X]$ and on its border with a given stepsize h . Additionally the nodes are assumed to be numbered increasingly x_0, x_1, \dots, x_N , where $N = X/h$, $x_0 = 0$ and $x_N = X$. Furthermore, we denote by y_m the approximation of $y(x_m)$ and equally $f_m = f(x_m, y_m)$ as discretized right hand side of the differential equation in question. In this setting we can formulate a definition of a linear multistep method:

Definition 2.2.3 We define a linear multistep method for an ordinary differential equation of first order (i.e. $n = 1$ in (2.5)) by

$$(2.8) \quad \sum_{k=-1}^p \alpha_k y_{m-k} = h \sum_{k=-1}^p \beta_k f(x_{m-k}, y_{m-k})$$

where α_k, β_k for $k = -1, 0, 1, \dots, p$ denote real constants.

Assigned to each linear multistep method are its first (ρ) and second (σ) characteristic polynomial. These are given by

$$(2.9) \quad \rho(\zeta) = \sum_{k=-1}^p \alpha_k \zeta^{p-k}$$

$$(2.10) \quad \sigma(\zeta) = \sum_{k=-1}^p \beta_k \zeta^{p-k}$$

From now on we will say linear multistep method of type (ρ, σ) to denote the structure of the method.

We have seen in Lemma 2.2.1 that ordinary differential equations are equivalent to a specific type of Volterra integral equation. Thus we are interested in the formulation of a linear multistep method (ρ, σ) applied to an integral equation.

Lemma 2.2.6 *A linear multistep method (ρ, σ) applied to the integral equation*

$$y(x) = \int_0^x f(t) dt,$$

can be described as convolution quadrature:

$$({}_h J f)(x) = h \sum_{j=0}^m \omega_{m-j} f(jh), \quad x = mh.$$

Here ${}_h J$ denotes the discretization of step length h for the integral operator J . The convolution weights ω_m are given by the power series of the generating function ω defined by

$$(2.11) \quad \omega(\zeta) = \frac{\sigma(1/\zeta)}{\rho(1/\zeta)}.$$

Proof: This lemma is a specific case of Lemma 2.1 in [93], which we will give in a later section.

A linear multistep method (ρ, σ) with p steps requires some knowledge of the solution at the points $y_i, i = 0, 1, \dots, p-1$ or otherwise the solution will not be uniquely determined and the linear multistep method will not work properly. In [70, Ch. 5.2-2] the question of existence and uniqueness of the solution of the approximating difference equation (2.8) is addressed.

The question of convergence of a numerical method for the solution of an ordinary differential equations is important for its applicability. In [70, Ch. 5.2-3] the following definition can be found.

Definition 2.2.4 *Let $f(x, y)$ defined for all $x \in [0, X]$ so that the initial value problem*

$$Dy(x) = f(x, y(x)); \quad y(0) = b_0$$

is uniquely solvable for all b_0 . A linear multistep method (ρ, σ) is then called convergent if

$$\lim_{\substack{h \rightarrow 0 \\ x_m = x}} y_m = y(x)$$

holds for all $x \in [0, X]$ and all solutions $\{y_m\}$ of the difference equation (2.8) having starting values y_0, \dots, y_{p-1} satisfying

$$\lim_{h \rightarrow 0} y_i = b_0, \quad i = 0, 1, \dots, p-1.$$

Convergence of a given linear multistep method is usually not proven directly but rather by proving that they are stable and consistent, which is equivalent to convergence as shown by Dahlquist in [27] and [28]. Stability and consistency can be defined as follows (see e.g. [96]):

Definition 2.2.5 1. A linear multistep method is stable, if and only if the corresponding convolution weights ω_m are bounded.

2. A linear multistep method is consistent of order p , if the following statement holds:

$$h\omega(e^{-h}) = 1 + O(h^p).$$

We finish this chapter with two examples of linear multistep methods, on the one hand the so called Adams method and on the other hand the backward difference formula. For both we will develop a fractional counterpart later on.

Example 2.2.1 (Adams-type) There exist two important types of Adams methods, the explicit type (Adams-Bashforth) and the implicit type (Adams-Moulton). Both have the same first characteristic polynomial, namely

$$\rho(\zeta) = \zeta^{p+1} - \zeta^p$$

but different second characteristic polynomials, which lead to two different difference equations:

$$y_{m+1} = y_m + h \sum_{k=0}^p \beta_k f(t_{m-k}, y_{m-k}) \quad (\text{Adams-Bashforth})$$

$$y_{m+1} = y_m + h \sum_{k=-1}^p \beta_k f(t_{m-k}, y_{m-k}) \quad (\text{Adams-Moulton})$$

The coefficients β_k of the second characteristic polynomial are usually chosen to maximize the accuracy. This can e.g. be done by “solving” the ordinary differential equation $y' = f(x, y(x))$ by integration, which leads in the discretized setting to

$$y(x_{m+1}) = y(x_m) + \int_{x_m}^{x_{m+1}} f(t, y(t)) dt = y(x_m) + \int_{x_m}^{x_{m+1}} F(t) dt.$$

In this identity the unknown function $F(t)$ is then replaced by its polynomial interpolation at the points t_{m-p}, \dots, t_m (Adams-Bashforth) or t_{m-p}, \dots, t_{m+1} (Adams-Moulton). Then the interpolating polynomial is readily integrated to obtain the Adams-type scheme.

Tables 2.1 and 2.2 show the results for the coefficients $\beta_k^{(p)}$ depending on the number of steps p used in the multistep method.

k	0	1	2	3	4	5
$\beta_k^{(0)}$	1					
$2\beta_k^{(1)}$	3	-1				
$12\beta_k^{(2)}$	23	-16	5			
$24\beta_k^{(3)}$	55	-59	37	-9		
$720\beta_k^{(4)}$	1901	-2774	2616	-1274	251	
$1440\beta_k^{(5)}$	4227	-7673	9482	-6798	2627	-425

Table 2.1: Adams-Bashforth coefficients of the second characteristic polynomial

k	-1	0	1	2	3	4
$\beta_k^{(0)}$	1					
$2\beta_k^{(1)}$	1	1				
$12\beta_k^{(2)}$	5	8	-1			
$24\beta_k^{(3)}$	9	19	-5	1		
$720\beta_k^{(4)}$	251	646	-264	106	-19	
$1440\beta_k^{(5)}$	475	1427	-798	482	-173	27

Table 2.2: Adams-Moulton coefficients of the second characteristic polynomial

Example 2.2.2 (Backward difference formula) *Instead of interpolation of the unknown function under the integral as in the case of the Adams-type methods we could just as easily interpolate the function $y'(x)$ on the left hand side of the ordinary differential equation $y'(x) = f(x, y(x))$, then differentiate it to match the problem and thus obtain the multistep method. This approach leads to a multistep method having the general form*

$$\sum_{k=-1}^p \alpha_k y_{m-k} = h f(x_{m+1}, y_{m+1})$$

where the “convolution” weights α_k can be described as the coefficients of a Maclaurin series of a corresponding generating function given by

$$(2.12) \quad \alpha(\zeta) = \sum_{k=0}^p \alpha_k \zeta^k = \sum_{k=1}^p \frac{1}{k} (1 - \zeta)^k.$$

Thus we get the following table for the coefficients $\alpha_k^{(p)}$ depending on the number of steps p used in the multistep method.

k	-1	0	1	2	3	4	5
$\alpha_k^{(0)}$	1						
$\alpha_k^{(1)}$	1	-1					
$2\alpha_k^{(2)}$	3	-4	1				
$6\alpha_k^{(3)}$	11	-18	9	-2			
$12\alpha_k^{(4)}$	25	-48	48	16	3		
$60\alpha_k^{(5)}$	137	-300	300	-200	75	-12	
$60\alpha_k^{(6)}$	147	-360	450	-400	225	-72	10

Table 2.3: Backward difference formula coefficients of the first characteristic polynomial

Chapter 3

Integral transforms and special functions

A frequently used tool in classical calculus are integral transforms. This statement holds true for the fractional calculus in Chapter 4 as well. Thus we refresh the definitions and properties of some results of those transforms in this chapter. Additionally, the generalization of classical (integer) calculus to fractional calculus is accompanied with generalizations of special functions, which are frequently used in important results of classical calculus. Such functions are inter alia Euler's Gamma function as generalization of the factorial or the Mittag-Leffler function. A number of the results in the following Chapter 4 on fractional calculus can be understood easier, if the generalization of these special functions are well understood. For this reason the next sections give an overview of the definition and properties of some special functions used in the fractional calculus.

3.1 Integral transforms

Definition 3.1.1 *Let $f(x)$ be a given function in a certain function space. Then the classical integral transform is given by*

$$(3.1) \quad (Kf)(x) = \int_{-\infty}^{\infty} k(x, t) f(t) dt = g(x),$$

where $k(x, t)$ is some given function (called the kernel of the transform) and g is the transform of the function f . The most important integral transforms are the Fourier transform, where

$$(3.2) \quad k(x, t) = e^{ixt}$$

and the Laplace transform, where

$$(3.3) \quad k(x, t) = \begin{cases} e^{-xt} & \text{if } t > 0 \\ 0 & \text{if } t \leq 0. \end{cases}$$

Remark 3.1.1 Using standard notation, we write for the Fourier transform of a function $f(x)$ of a real variable $-\infty < x < \infty$

$$\mathcal{F}f = (\mathcal{F}f)(x) = \mathcal{F}\{f(t); x\} = \hat{f}(x) = \int_{-\infty}^{\infty} e^{ixt} f(t) dt,$$

and the Laplace transform of a function $f(x)$, $0 < x < \infty$ as

$$\mathcal{L}f = (\mathcal{L}f)(p) = \mathcal{L}\{f(t), p\} = \int_0^{\infty} e^{-pt} f(t) dt.$$

The advantage of integral transforms can often be seen by the fact that a mathematical problem is easier to solve, if it is first *translated* by the integral transform and then solved in the new domain. However, the result is often needed in the original domain so that the existence of an inverse integral transform is essential. For the Fourier and Laplace transform those are given in the following definition:

Definition 3.1.2 Let $f(x)$ be a given function in a certain function space. Then the inverse Fourier transform is defined as

$$(3.4) \quad (\mathcal{F}^{-1}f)(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ixt} f(t) dt.$$

The inverse of the Laplace transform (also known as Bromwich integral) is defined as

$$(3.5) \quad (\mathcal{L}^{-1}f)(x) = \mathcal{L}^{-1}\{f(p); x\} = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{px} f(p) dp,$$

where the integration is done along the vertical line $x = \gamma$ in the complex plane such that γ is greater than the real part of all singularities of $f(p)$.

In connection with the stated integral transform the idea (and properties) of convolution of two functions is quite useful:

Definition 3.1.3 Let $f, g \in L_1(\mathbb{R})$. The Fourier convolution of f and g is denoted by $f * g$ and defined as

$$(f * g)(x) := \int_{-\infty}^{\infty} f(x-t)g(t)dt, \quad x \in \mathbb{R}.$$

The Laplace convolution of f and g is denoted by $f * g$ and defined as

$$(f * g)(x) := \int_0^x f(x-t)g(t)dt, \quad x > 0.$$

Both the Laplace and the Fourier convolution of two functions f and g are denoted by $f * g$. Thus one has to specify which convolution is used in any given context. However, both convolutions satisfy the following properties:

Theorem 3.1.1 Let $f, g, h \in L_1(\mathbb{R})$ and $a \in \mathbb{C}$. Then the following properties hold:

1. Commutativity, i.e. $f * g = g * f$,
2. Associativity, i.e. $f * (g * h) = (f * g) * h$,
3. Distributivity, i.e. $f * (g + h) = f * g + f * h$,
4. Associativity with scalar multiplication, i.e. $a(f * g) = (af) * g = f * (ag)$.

The two stated integral transforms exhibit important features regarding the convolution of two functions f and g :

Theorem 3.1.2 (Convolution Theorem) Let f, g be two functions for which the Fourier (Laplace) transform exist. Then, respectively

$$\mathcal{F}(f * g)(x) = \sqrt{2\pi} \mathcal{F}(f)(x) \cdot \mathcal{F}(g)(x) \quad \text{and} \quad \mathcal{L}(f * g)(x) = \mathcal{L}(f)(x) \cdot \mathcal{L}(g)(x),$$

i.e. the Fourier (Laplace) convolution of two functions becomes a simple product in the Fourier (Laplace) domain.

3.2 Euler's Gamma function

In the study of special functions a fundamental cornerstone is given by Euler's Gamma function. The reason herein lies in the fact that this function can be encountered in nearly all parts of the subject and furthermore many special functions can be expressed in term of the Gamma functions directly or by contour integration. Before we give a formal definition of Euler's Gamma function we need an additional definition, which will be used in the proofs for some properties of the Gamma function.

Definition 3.2.1 The Euler constant γ is given by

$$(3.6) \quad \gamma = \lim_{n \rightarrow \infty} \left(\sum_{k=1}^n \frac{1}{k} - \ln(n) \right) \approx 0.5772156649.$$

The Euler constant is also known as Euler-Mascheroni constant.

There are a number of ways, how Euler's Gamma function can be defined. We give the one, which will be most useful for our later considerations in fractional calculus.

Definition 3.2.2 For $z \in \mathbb{C} \setminus \{0, -1, -2, -3, \dots\}$ Euler's Gamma function $\Gamma(z)$ is defined as

$$(3.7) \quad \Gamma(z) = \begin{cases} \int_0^\infty t^{z-1} e^{-t} dt, & \text{if } \operatorname{Re}(z) > 0 \\ \Gamma(z+1)/z, & \text{if } \operatorname{Re}(z) \leq 0, \quad z \neq 0, -1, -2, -3, \dots \end{cases}$$

Euler's Gamma function is defined in the whole complex plane except zero and negative integers, where Euler's Gamma function has poles; the values in $(-1, 0)$ are uniquely given by the ones from $(0, 1)$, the values in $(-2, -1)$ are uniquely defined by the ones in $(-1, 0)$ and so on. Next we state some properties of Euler's Gamma function, which will become useful in later chapters.

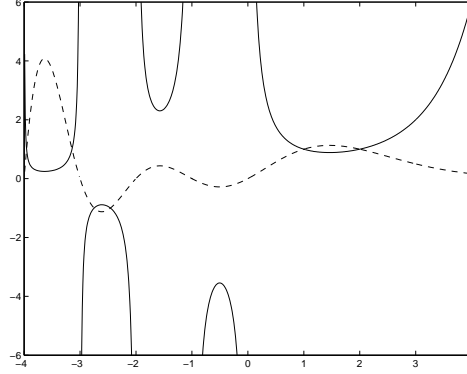


Figure 3.1: Euler's Gamma function $\Gamma(z)$ (solid) and its reciprocal (dashed) on the interval $(-4, 4]$.

Theorem 3.2.1 *Euler's Gamma function satisfies the following properties:*

1. For $\operatorname{Re}(z) > 0$, the first part of definition (3.7) is equivalent to

$$\Gamma(z) = \int_0^1 \left(\ln \left(\frac{1}{t} \right) \right)^{z-1} dt.$$

2. For $z \in \mathbb{C} \setminus \{0, -1, -2, -3, \dots\}$

$$\Gamma(1+z) = z\Gamma(z).$$

3. For $n \in \mathbb{N}$

$$\Gamma(n) = (n-1)!.$$

4. For $z \in \mathbb{C} \setminus \{0, 1, 2, 3, \dots\}$

$$\Gamma(1-z) = -z\Gamma(-z).$$

5. (Limit representation) For $\operatorname{Re}(z) > 0$ the following limit holds:

$$(3.8) \quad \Gamma(z) = \lim_{n \rightarrow \infty} \frac{n!n^z}{z(z+1)(z+2)\dots(z+n)}$$

The Limit representation is equivalent to Euler's infinite product, given by

$$\frac{1}{z} \prod_{n=1}^{\infty} \frac{(1 + (1/n))^z}{1 + (z/n)}.$$

6. (Weierstrass definition) Let $z \in \mathbb{C} \setminus \{0, -1, -2, -3, \dots\}$. Then Euler's Gamma function can be defined by

$$\frac{1}{\Gamma(z)} = ze^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n} \right) e^{-z/n},$$

where γ is the Euler constant (3.6).

7. Euler's Gamma function is analytic for all $z \in \mathbb{C} \setminus \{0, -1, -2, -3, \dots\}$

8. Euler's Gamma function is never zero.

9. (Reflection Theorem) For all non-integer $z \in \mathbb{C}$,

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}, \quad \text{and} \quad \Gamma(z)\Gamma(-z) = -\frac{\pi}{z \sin(\pi z)}$$

10. For half-integer arguments, $\Gamma(n/2)$, $n \in \mathbb{N}$ has the special form

$$\Gamma(n/2) = \frac{(n-2)!!\sqrt{\pi}}{2^{(n-1)/2}},$$

where $n!!$ is the double factorial:

$$n!! = \begin{cases} n \cdot (n-2) \dots 5 \cdot 3 \cdot 1 & n > 0 \text{ odd} \\ n \cdot (n-2) \dots 6 \cdot 4 \cdot 2 & n > 0 \text{ even} \\ 1 & n = 0, -1 \end{cases}$$

Proof: The first four properties can be proven easily: 1 follows by a simple change of variable ($u = -\log(t)$). Integration by parts of the integral in (3.7) yields

$$\begin{aligned} \Gamma(z) &= \int_0^\infty t^{z-1} e^{-t} dt = [-t^{z-1} e^{-t}]_0^\infty + \int_0^\infty (z-1) t^{z-2} e^{-t} dt \\ &= (z-1) \int_0^\infty t^{z-2} e^{-t} dt = (z-1) \Gamma(z-1) \end{aligned}$$

and thus gives the second property. It is easily seen that $\Gamma(1) = 1$ and thus repeated application of the property 2 yields property 3. The fourth property follows from the second one (and in fact gives the definition of Euler's Gamma function in the left-hand complex plane explained above).

In order to prove the property 5, we introduce the auxiliary function

$$\Gamma_n(z) = \int_0^n \left(1 - \frac{t}{n}\right)^n t^{z-1} dt.$$

For this function, integration by parts with the substitution $s = t/n$ yields

$$\begin{aligned} \Gamma_n(z) &= n^z \int_0^1 (1-s)^n s^{z-1} ds \\ &= \frac{n^z}{z} \int_0^1 (1-s)^{n-z} s^z ds \\ &= \frac{n! n^z}{z(z+1)(z+2) \dots (z+n-1)} \int_0^1 s^{z+n-1} ds \\ &= \frac{n! n^z}{z(z+1)(z+2) \dots (z+n)}, \end{aligned}$$

which is equation (3.8) in property 5. The equivalence of the limit of the auxiliary function with Euler's Gamma function is deduced by using the limit

$$\lim_{n \rightarrow \infty} \left(1 - \frac{t}{n}\right)^n = e^{-t}$$

and thus concluding that

$$\lim_{n \rightarrow \infty} \Gamma_n(z) = \lim_{n \rightarrow \infty} \int_0^n \left(1 - \frac{t}{n}\right)^n t^{z-1} dt = \int_0^\infty e^{-t} t^{z-1} dt,$$

given that the limit and the integral are interchangeable (a proof of this can be found in [122, pp.5-7]) and the limit of the term under the integral exists (which is a standard result of analysis). A proof of the equivalence of equation (3.8) with Euler's infinite product then follows by simple calculations.

The auxiliary function $\Gamma_n(z)$ can also be used to prove property 6. We note that

$$\begin{aligned} \Gamma_n(z) &= \frac{n!n^z}{z(z+1)(z+2)\dots(z+n)} \\ &= \frac{n^z}{z(1+z/1)(1+z/2)\dots(1+z/n)}. \end{aligned}$$

Using the relation

$$n^z = e^{z \ln(n)} = e^{z(\ln(n)-1-1/2-\dots-1/n)} e^{z+z/2+\dots+z/n}$$

we can then conclude that

$$\begin{aligned} \Gamma_n(z) &= \frac{e^{z(\ln(n)-1-1/2-\dots-1/n)} e^{z+z/2+\dots+z/n}}{z(1+z)(1+z/2)\dots(1+z/n)} \\ &= e^{z(\ln(n)-1-1/2-\dots-1/n)} \frac{1}{z} \frac{e^z}{(1+z)} \frac{e^{z/2}}{(1+z/2)} \dots \frac{e^{z/n}}{(1+z/n)}. \end{aligned}$$

With the limit representation 5, property 6 follows by

$$\begin{aligned} \frac{1}{\Gamma(z)} &= \lim_{n \rightarrow \infty} \frac{1}{\Gamma_n(z)} \\ &= e^{z\gamma} z \lim_{n \rightarrow \infty} e^{-z} (1+z) e^{-z/2} (1+z/2) \dots e^{-z/n} (1+z/n) \\ &= z e^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right) e^{-z/n}. \end{aligned}$$

Having established a proof for property 6, properties 7 and 8 follow immediately: Weierstrass' definition is analytic for all finite z and its only zeros are simple ones at $z = 0$ and each negative integer. Thus $\Gamma(z)$ is analytic except at the non-positive integers and at $z = \infty$. Additionally $\Gamma(z)$ is never zero since $1/\Gamma(z)$ has no poles.

The Weierstrass definition gives us also a nice way to prove the reflection Theorem 9. Starting with

$$\begin{aligned}\frac{1}{\Gamma(z)} \frac{1}{\Gamma(-z)} &= -z^2 e^{\gamma z} e^{-\gamma z} \prod_{n=1}^{\infty} \left[\left(1 + \frac{z}{n}\right) e^{-z/n} \left(1 - \frac{z}{n}\right) e^{z/n} \right] \\ &= -z^2 \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2}\right)\end{aligned}$$

we can utilize the functional equation 4 to gain

$$\frac{1}{\Gamma(z)} \frac{1}{\Gamma(1-z)} = z \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2}\right)$$

and with the series expansion

$$\sin(\pi z) = \pi z \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2}\right)$$

for the sine function we finally get

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi x)}.$$

The second identity in 9 can be deduced analogously. A proof for property 10 can be found in [5]. □

Many additional properties of Euler's Gamma function can be found in a number of books on special functions, such as [6, 22, 49, 50, 51, 100, 101, 126]. But for the following chapters the stated properties will be sufficient. However, there are a number of interesting consequences to be drawn from Theorem 3.2.1:

- From property 3 it becomes obvious that Euler's Gamma function is a generalization of the factorial.
- The values in the left complex plane are defined by property 2 and the poles explain the fact that the definition excludes numbers whose real part is zero or a negative integer. The appearance of poles at those numbers can be explained by property 2 as well (since all applicable intervals on the left complex plane use the values of the Gamma function near zero on both interval ends by recursion).
- By induction property 4 can easily be generalized to

$$\Gamma(n-x) = (-1)^n \Gamma(-x) \prod_{j=0}^{n-1} (x-j),$$

with $n \in \mathbb{N}$ and $x \in \mathbb{C} \setminus \{0, 1, 2, \dots\}$.

- Combining property 9 and property 4 we get

$$\Gamma(-z)\Gamma(z+1) = \frac{\Gamma(1-z)}{-z}\Gamma(z)z = -\Gamma(1-z)\Gamma(z) = -\frac{\pi}{\sin(\pi z)}$$

or more general for $k \in \mathbb{N}_0$:

$$(-1)^{k+1}\Gamma(z-k)\Gamma(k+1-z) = \Gamma(-z)\Gamma(z+1).$$

Sometimes the last equation is stated as the reflection formula instead of property 9.

- Property 10 gives a number of values for the Gamma function which often occur in classical applications. The first half-integer values of the Euler's Gamma function are given by:

α	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$	$\frac{13}{2}$
$\Gamma(\alpha)$	$\sqrt{\pi}$	$\frac{1}{2}\sqrt{\pi}$	$\frac{3}{4}\sqrt{\pi}$	$\frac{15}{8}\sqrt{\pi}$	$\frac{105}{16}\sqrt{\pi}$	$\frac{945}{32}\sqrt{\pi}$	$\frac{10395}{64}\sqrt{\pi}$

Directly connected to Euler's Gamma function is the definition of generalized binomial coefficients:

Definition 3.2.3 The generalized binomial coefficients $\binom{\alpha}{k}$ for $\alpha \in \mathbb{R}$ and $k \in \mathbb{N}_0$ are defined by

$$\binom{\alpha}{k} = \frac{(-1)^{k-1}\Gamma(k-\alpha)}{\Gamma(1-\alpha)\Gamma(k+1)} = \frac{\alpha(\alpha-1)(\alpha-2)\cdots(\alpha-k+1)}{k!}.$$

With the help of Euler's Gamma function a number of additional special functions can be defined and some of those are useful in the generalization of classical calculus to its fractional counterpart. Therefore, we state some other special functions, starting with the Beta function.

3.3 The Beta function

A special function, which is connected to Euler's Gamma function in a direct way, is given by the Beta function, defined as follows:

Definition 3.3.1 The Beta function $B(p, q)$ in two variables $p, q \in \mathbb{C}$ is defined by

$$(3.9) \quad B(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}$$

Again we state some properties of this special function, which we will use later on. Especially the *Beta integral* in the following theorem will be used for examples in the chapter on fractional calculus.

Theorem 3.3.1 *The Beta function possesses the following properties:*

1. For $\operatorname{Re}(z), \operatorname{Re}(w) > 0$, the definition (3.9) is equivalent to

$$(3.10) \quad B(z, w) = \int_0^1 t^{z-1} (1-t)^{w-1} dt = \int_0^\infty \frac{t^{z-1}}{(1+t)^{z+w}} dt$$

$$(3.11) \quad = 2 \int_0^{\pi/2} (\sin t)^{2z-1} (\cos t)^{2w-1} dt.$$

2. $B(z+1, w+1)$ is the solution of the Beta Integral :

$$\int_0^1 t^z (1-t)^w dt = B(z+1, w+1).$$

3. The following identities hold:

$$(a) \quad B(z, w) = B(w, z),$$

$$(b) \quad B(z, w) = B(z+1, w) + B(z, w+1),$$

$$(c) \quad B(z, w+1) = \frac{w}{z} B(z+1, w) = \frac{w}{z+w} B(z, w).$$

Proof: We first note that the stated equality on the right-hand side of (3.10) in property 1 indeed holds. For this we substitute $t = x/(x+1)$, obtaining

$$\int_0^\infty \frac{x^{z-1}}{(1+x)^{z+w}} dx,$$

which by renaming the variables proves the equality. In the same manner we obtain (3.11) by setting $t = \sin^2 \varphi$ in the middle term of (3.10):

$$\int_0^1 t^{z-1} (1-t)^{w-1} dt = \int_0^{\pi/2} \sin^{2z-1} \varphi \cos^{2w-1} \varphi d\varphi,$$

which immediately recovers the term (3.11). At last, the connection with the representation using Euler's Gamma functions can be derived as follows: Consider the product

$$\Gamma(z)\Gamma(w) = \int_0^\infty e^{-t} t^{z-1} dt \int_0^\infty e^{-s} s^{w-1} ds$$

and set $t = x^2, s = y^2$ to obtain

$$\begin{aligned} \Gamma(z)\Gamma(w) &= 4 \int_0^\infty e^{-x^2} x^{2z-1} dx \int_0^\infty e^{-y^2} y^{2w-1} dy \\ &= 4 \int_0^\infty \int_0^\infty e^{-x^2-y^2} x^{2z-1} y^{2w-1} dx dy. \end{aligned}$$

Using polar coordinates $x = r \cos \theta$, $y = r \sin \theta$ we can then write

$$\begin{aligned}\Gamma(z)\Gamma(w) &= 4 \int_0^\infty \int_0^{\pi/2} e^{-r^2} r^{2z+2w-2} (\cos \theta)^{2z-1} (\sin \theta)^{2w-1} r d\theta dr \\ &= 2 \int_0^\infty e^{-r^2} r^{2z+2w-1} dr \times 2 \int_0^{\pi/2} (\cos \theta)^{2z-1} (\sin \theta)^{2w-1} d\theta\end{aligned}$$

and with the resubstitution $r = \sqrt{t}$ and $\theta = \pi/2 - \varphi$ we finally get

$$\Gamma(z)\Gamma(w) = \int_0^\infty e^{-t} t^{z+w-1} dt \times 2 \int_0^{\pi/2} (\sin \varphi)^{2z-1} (\cos \varphi)^{2w-1} d\varphi.$$

From the last statement it follows that $\Gamma(z)\Gamma(w) = \Gamma(z+w)B(z, w)$ and thus property 1.

The second property is just a rewritten version of property 1, which is stated here because of its significance later on. The three identities in property 3 can easily be proven using one of the representations of the first property. \square

We will use the Beta function, and more importantly the fact that we can use it to describe the solution of the Beta integral, for a number of examples later on. For its usefulness from a more analytical point of view, we will next define the Mittag-Leffler function, which again is strongly connected to Euler's Gamma function.

3.4 Mittag-Leffler function

Definition 3.4.1 For $z \in \mathbb{C}$ the Mittag-Leffler Function $E_\alpha(z)$ is defined by

$$(3.12) \quad E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \alpha > 0$$

and the generalized Mittag-Leffler Function $E_{\alpha,\beta}(z)$ by

$$(3.13) \quad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta > 0.$$

In the following theorem we state some of the properties of the Mittag-Leffler function, which will be of some use later on in the analysis of ordinary as well as partial differential equations of fractional order.

Theorem 3.4.1 The Mittag-Leffler function possesses the following properties:

1. For $|z| < 1$ the generalized Mittag-Leffler function satisfies

$$\int_0^\infty e^{-t} t^{\beta-1} E_{\alpha,\beta}(t^\alpha z) dt = \frac{1}{z-1}.$$

2. For $|z| < 1$, the Laplace transform of the Mittag-Leffler function $E_\alpha(z^\alpha)$ is given by

$$\int_0^\infty e^{-zt} E_\alpha(z^\alpha) dt = \frac{1}{z - z^{1-\alpha}}$$

3. The Mittag-Leffler function (3.12) converges for every $z \in \mathbb{C}$.

4. For special values α the Mittag-Leffler function is given by:

$$\begin{aligned} (a) E_0(z) &= \frac{1}{1-z} & (b) E_1(z) &= e^z \\ (c) E_2(z^2) &= \cosh(z) & (d) E_2(-z^2) &= \cos(z) \end{aligned}$$

Proof: To prove property 1, we first deduce the Laplace transform of a function $t^k e^{qt}$. For this we first use the series expansion of $\exp(z)$ and the definition of Euler's Gamma function to show that

$$\int_0^\infty e^{-t} e^{zt} dt = \sum_{k=0}^\infty \frac{z^k}{k!} \int_0^\infty e^{-t} t^k dt = \sum_{k=0}^\infty z^k = \frac{1}{1-z}$$

holds for $|z| < 1$. Differentiating this statement k times with respect to z yields

$$\int_0^\infty e^{-t} t^k e^{zt} dt = \frac{k!}{(1-z)^{k+1}}, \quad |z| < 1.$$

Substituting $z = 1 + q - p$ we then get the Laplace transform of the function $t^k e^{qt}$:

$$\int_0^\infty e^{-pt} t^k e^{qt} dt = \frac{k!}{(q-p)^{k+1}}, \quad \operatorname{Re}(p) > |q|.$$

If we now consider the Laplace transform of the Mittag-Leffler function, we can argue in the same manner as above:

$$\begin{aligned} \int_0^\infty e^{-t} t^{\beta-1} E_{\alpha,\beta}(zt^\alpha) dt &= \int_0^\infty e^{-t} t^{\beta-1} \sum_{k=0}^\infty \frac{(zt^\alpha)^k}{\Gamma(\alpha k + \beta)} dt \\ &= \frac{1}{1-z}, \quad |z| < 1. \end{aligned}$$

A proof for property 2 can be found in [51] and property 3 follows from the definition of the Mittag-Leffler function and the knowledge of corresponding series expansions of the stated functions. \square

In Figure 3.2 we have plotted the Mittag-Leffler function $E_\alpha(-z^\alpha)$ for different values of α . We have chosen a negative argument in order to clarify the connection between the Mittag-Leffler function and the exponential functions as well as the cosine, which will become of greater importance in the fractional formulation of the classical diffusion-wave equation in Chapter 6.2.

Remark 3.4.1 The Mittag-Leffler function is related to the generalized hypergeometric function $F_{n,r}^\beta(z)$, defined as

$$(3.14) \quad F_{n,r}^\beta(z) := \sum_{k=0}^\infty \frac{\beta^k}{(nk+r)!} z^{nk+r}$$

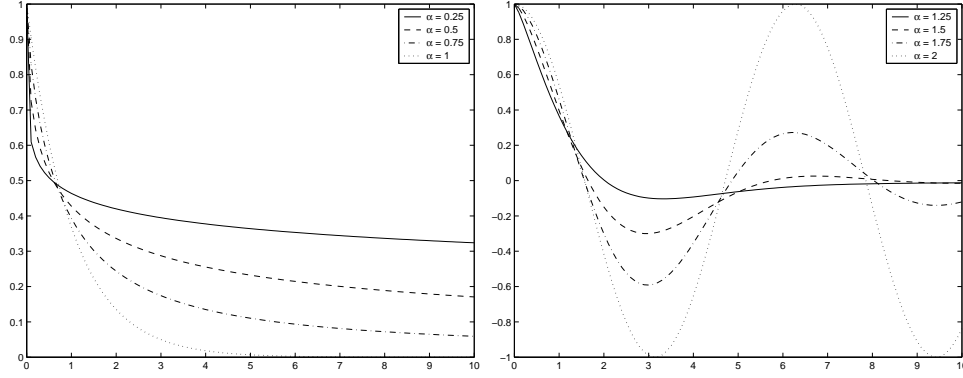


Figure 3.2: Mittag-Leffler Function $E_\alpha(-z^\alpha)$ for different values of α .

and to the confluent hypergeometric function ${}_1F_1(a; b; z)$, also known as Kummer's function of the first kind and defined as

$$(3.15) \quad {}_1F_1(a; b; z) := \sum_{k=0}^{\infty} \frac{\Gamma(a+k)}{\Gamma(a)} \frac{\Gamma(b)}{\Gamma(b+k)} \frac{z^k}{k!}.$$

With this chapter on integral transforms and special functions we leave the field of classical integer calculus and move forward to the new field of fractional calculus.

Chapter 4

Fractional calculus

In Chapter 1 a brief history of fractional calculus has been presented and the strong connection with the development of classical calculus was established. Moreover, some analytical results and applications of fractional calculus have been outlined in their historical context. In this chapter a structured view on the analysis of non-integer order calculus will be presented. As in Chapter 2 we will look into aspects of integration and differentiation, differential equations and partial differential equations separately. The results of this chapter are in greater parts well known and can be found in various books [105, 110, 122, 141] on fractional calculus. Additionally there exists a lecture-script by K. Diethelm [33], from which a number of the results and proofs in this chapter were taken.

4.1 Fractional integration and differentiation

As seen in the historical outline in Chapter 1, more than one way to transfer integer-order operations to the non-integer case was developed. Therefore, we divide this section into a number of subsections, each dealing with one set of operations. We start with the most common one, the Riemann-Liouville operators for fractional differentiation and integration.

4.1.1 Riemann-Liouville operator

Replacing $n \in \mathbb{N}$ with $\alpha \in \mathbb{R}$ in Lemma 2.1.2 and using Euler's Gamma function (3.7) instead of the factorial we obtain the following definition:

Definition 4.1.1 *Let $\alpha \in \mathbb{R}_+$. The operator J_a^α , defined on $L_1[a, b]$ by*

$$(4.1) \quad J_a^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) dt$$

for $a \leq x \leq b$, is called the Riemann-Liouville fractional integral operator of order α . For $\alpha = 0$, we set $J_a^0 := I$, the identity operator.

By construction it is obvious that for $\alpha \in \mathbb{N}$ the Riemann-Liouville integral coincides with the classical integral J_a^n in Definition 2.1.1 except that the domain has been extended from Riemann integrable to Lebesgue integrable functions. The existence of the integral in Definition 4.1.1 is assured for the case $\alpha \geq 1$ by the fact that the integrand is the product of an integrable function f and the continuous function $(x - \cdot)^{\alpha-1}$. The existence for the case $\alpha \in (0, 1)$ is addressed in the following theorem:

Theorem 4.1.1 *Let $f \in L_1[a, b]$ and $\alpha > 0$. Then the integral $J_a^\alpha f(x)$ exists for almost every $x \in [a, b]$ and the function $J_a^\alpha f$ itself is also an element of $L_1[a, b]$.*

Proof: We write the integral in question as

$$\int_a^x (x-t)^{\alpha-1} f(t) dt = \int_{-\infty}^{\infty} \phi_1(x-t) \phi_2(t) dt$$

where

$$\phi_1(u) = \begin{cases} u^{\alpha-1} & \text{for } 0 < u \leq b-a, \\ 0 & \text{else,} \end{cases}$$

and

$$\phi_2(u) = \begin{cases} f(u) & \text{for } a \leq u \leq b, \\ 0 & \text{else.} \end{cases}$$

By construction, $\phi_j \in L_1(\mathbb{R})$ for $j \in \{1, 2\}$, and thus by a classical result on Lebesgue integration [152, Thm. 4.2d] the desired result follows. \square

With the existence of the fractional integral of Definition 4.1.1 guaranteed, the first question to be answered is, which aspects known for the integer order integrals carry over to the Riemann-Liouville fractional integral. A first result is given by the following theorem:

Theorem 4.1.2 *The operators $\{J_a^\alpha : L_1[a, b] \rightarrow L_1[a, b]; \alpha \geq 0\}$ form a commutative semigroup with respect to concatenation. The identity operator J_a^0 is the neutral element of this semigroup.*

This algebraically formulated result implies directly

$$(4.2) \quad J_a^\alpha J_a^\beta f = J_a^{\alpha+\beta} f = J_a^{\beta+\alpha} f = J_a^\beta J_a^\alpha f,$$

if $f \in L_1[a, b]$, $\alpha, \beta \in \mathbb{R}_+$, which is a well known result in the integer case.

Proof: The neutral element of the semigroup is ascertained by Definition 4.1.1. Therefore, we only need to prove that relation (4.2) holds almost everywhere. By definition of the fractional integral we have

$$J_a^\alpha J_a^\beta f(x) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x (x-t)^{\alpha-1} \int_a^t (t-\tau)^{\beta-1} f(\tau) d\tau dt.$$

In view of Theorem 2.1.4, the integrals exist, and by Fubini's Theorem 2.1.11 we may interchange the order of integration, obtaining

$$\begin{aligned} J_a^\alpha J_a^\beta f(x) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \int_\tau^x (x-t)^{\alpha-1} (t-\tau)^{\beta-1} f(\tau) dt d\tau \\ &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x f(\tau) \int_\tau^x (x-t)^{\alpha-1} (t-\tau)^{\beta-1} dt d\tau. \end{aligned}$$

The substitution $t = \tau + s(x - \tau)$ yields

$$\begin{aligned} J_a^\alpha J_a^\beta f(x) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x f(\tau) \int_0^1 [(x-\tau)(1-s)]^{\alpha-1} \\ &\quad \times [s(x-\tau)]^{\beta-1} (x-\tau) ds d\tau \\ &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x f(\tau) (x-\tau)^{\alpha+\beta-1} \int_0^1 (1-s)^{\alpha-1} s^{\beta-1} ds d\tau. \end{aligned}$$

The term $\int_0^1 (1-s)^{\alpha-1} s^{\beta-1} ds$ is the Beta function (see Definition 3.3.1), and thus

$$J_a^\alpha J_a^\beta f(x) = \frac{1}{\Gamma(\alpha+\beta)} \int_a^x f(\tau) (x-\tau)^{\alpha+\beta-1} d\tau = J_a^{\alpha+\beta} f(x)$$

holds almost everywhere on $[a, b]$. □

Next we look at mapping properties of the fractional integral operator J_a^α , which will be useful for later theorems. A number of such properties can be found in [141], but we restrict ourselves to two results, one for the Hölder spaces and one for the Lebesgue spaces. Proofs of both theorems can be found in [33, Thm. 2.5 and 2.6].

Theorem 4.1.3 *Let $f \in H_\mu[a, b]$ for some $\mu \in [0, 1]$, and let $0 < \alpha < 1$. Then*

$$J_a^\alpha f(x) = \frac{f(a)}{\Gamma(\alpha+1)} (x-a)^\alpha + \Phi(x)$$

with some function Φ . This function Φ satisfies

$$\Phi(x) = O((x-a)^{\mu+\alpha})$$

as $x \rightarrow a$. Moreover,

$$\Phi \in \begin{cases} H_{\mu+\alpha}[a, b] & \text{if } \mu + \alpha < 1, \\ H^*[a, b] & \text{if } \mu + \alpha = 1, \\ H_1[a, b] & \text{if } \mu + \alpha > 1. \end{cases}$$

Theorem 4.1.4 *Let $\alpha > 0$, $p > \max\{1, 1/\alpha\}$, and $f \in L_p[a, b]$. Then*

$$J_a^\alpha f(x) = o((x-a)^{\alpha-1/p})$$

as $x \rightarrow a+$. If additionally $\alpha - 1/p \notin \mathbb{N}$, then $J_a^\alpha f \in C^{[\alpha-1/p]}[a, b]$, and $D^{[\alpha-1/p]} J_a^\alpha f \in H_{\alpha-1/p-[\alpha-1/p]}[a, b]$.

As next topic we discuss the interchangeability of limit operation and fractional integration. For the classical case $\alpha \in \mathbb{N}$, it is well known that those two operations are interchangeable. The following theorem states a similar result for the fractional case:

Theorem 4.1.5 *Let $\alpha > 0$. Assume that $(f_k)_{k=1}^\infty$ is a uniformly convergent sequence of continuous functions on $[a, b]$. Then we may interchange the fractional integral operator and the limit process, i.e.*

$$\left(J_a^\alpha \lim_{k \rightarrow \infty} f_k \right) (x) = \left(\lim_{k \rightarrow \infty} J_a^\alpha f_k \right) (x).$$

In particular, the sequence of functions $(J_a^\alpha f_k)_{k=1}^\infty$ is uniformly convergent.

Proof: For the first statement we utilize the well known fact, that if f denotes the limit of the sequence (f_k) , the function f is continuous. For $\alpha = 0$ the stated result follows directly from the uniform convergence and for $\alpha > 0$ we can deduce

$$\begin{aligned} |J_a^\alpha f_k(x) - J_a^\alpha f(x)| &\leq \frac{1}{\Gamma(\alpha)} \int_a^x |f_k(t) - f(t)| (x-t)^{\alpha-1} dt \\ &\leq \frac{1}{\Gamma(\alpha+1)} \|f_k - f\|_\infty (b-a)^\alpha. \end{aligned}$$

The last term converges uniformly to zero as $k \rightarrow \infty$ for all $x \in [a, b]$. □

A direct consequence of this theorem points out the connection between fractional integrals and integer-order derivatives of an analytic function.

Corollary 4.1.6 *Let f be analytic in $(a-h, a+h)$ for some $h > 0$, and let $\alpha > 0$. Then*

$$J_a^\alpha f(x) = \sum_{k=0}^{\infty} \frac{(-1)^k (x-a)^{k+\alpha}}{k! (\alpha+k) \Gamma(\alpha)} D^k f(x)$$

for $a \leq x < a+h/2$, and

$$J_a^\alpha f(x) = \sum_{k=0}^{\infty} \frac{(x-a)^{k+\alpha}}{\Gamma(k+1+\alpha)} D^k f(a)$$

for $a \leq x < a+h$. In particular, $J_a^\alpha f$ is analytic in $(a, a+h)$.

Before we prove this corollary we give an example for the fractional integration of a power function, which will be useful for the proof of Corollary 4.1.6 as well as for later applications.

Example 4.1.1 *Let $f(x) = (x-a)^c$ for some $c > -1$ and $\alpha > 0$. Then,*

$$J_a^\alpha f(x) = \frac{\Gamma(c+1)}{\Gamma(\alpha+c+1)} (x-a)^{\alpha+c}.$$

For the classical case $\alpha \in \mathbb{N}$ this is a well known result, and thus it is precisely what one would want from the generalization to the fractional case. This result can be obtained directly using the definition of Euler's Beta function (see Definition 3.3.1).

$$\begin{aligned} J_a^\alpha f(x) &= \frac{1}{\Gamma(\alpha)} \int_a^x (t-a)^c (x-t)^{\alpha-1} dt \\ &= \frac{1}{\Gamma(\alpha)} (x-a)^{\alpha+c} \int_0^1 s^\beta (1-s)^{\alpha-1} ds \\ &= \frac{\Gamma(c+1)}{\Gamma(\alpha+c+1)} (x-a)^{\alpha+c} \end{aligned}$$

Proof: (of Corollary 4.1.6) Since f is analytic, we can expand it into a power series about x . Furthermore, $x \in [a, a+h/2)$ and thus the power series converges in the entire interval of integration. By Theorem 4.1.5 we can exchange summation and integration. Then, using the explicit representation for the fractional integral of the power function from Example 4.1.1, the first statement follows. The second statement can be deduced in the same way by expanding the power series at a instead of x . The analyticity of $J_a^\alpha f$ follows immediately from the second statement. \square

Until now we only considered the Riemann-Liouville *integral* operator, which was motivated by a generalization of the result in Theorem 2.1.2. Recalling Theorem 2.1.3, which stated (under certain conditions) the identity

$$D^n f = D^m J_a^{m-n} f$$

for the integers m and n , we can now motivate the definition of the fractional *differential* operator by generalizing this identity to non-integer order:

Definition 4.1.2 Let $\alpha \in \mathbb{R}_+$ and $n = \lceil \alpha \rceil$. The operator D_a^α , defined by

$$(4.3) \quad D_a^\alpha f(x) = D^n J_a^{n-\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dx} \right)^n \int_a^x (x-t)^{n-\alpha-1} f(t) dt$$

for $a \leq x \leq b$, is called the Riemann-Liouville differential operator of order α . For $\alpha = 0$, we set $D_a^0 := I$, the identity operator.

As a first consequence of this definition we note, that if $\alpha \in \mathbb{N}$, the operator D_a^α in Definition 4.1.2 coincides with the classical differential operator D^n . Furthermore, we obtain a similar result to the one in Theorem 2.1.3 for the fractional case.

Lemma 4.1.7 Let $\alpha \in \mathbb{R}_+$ and let $n \in \mathbb{N}$ such that $n > \alpha$. Then,

$$D_a^\alpha = D^n J_a^{n-\alpha}.$$

Proof: The assumption on n implies that $n \geq \lceil \alpha \rceil$. Thus,

$$D^n J_a^{n-\alpha} = D^{\lceil \alpha \rceil} D^{n-\lceil \alpha \rceil} J_a^{n-\lceil \alpha \rceil} J_a^{\lceil \alpha \rceil - \alpha} = D^{\lceil \alpha \rceil} J_a^{\lceil \alpha \rceil - \alpha} = D_a^\alpha$$

in view of the semigroup property of fractional integration and the fact that ordinary differentiation is left-inverse to integer integration. \square

As for the Riemann-Liouville integral operator, we have to assure the existence of the fractional derivative of a given function under certain conditions. The following result states a simple sufficient condition for the existence of $D_a^\alpha f$:

Lemma 4.1.8 *Let $f \in A^1[a, b]$ and $0 < \alpha < 1$. Then $D_a^\alpha f$ exists almost everywhere in $[a, b]$. Moreover, $D_a^\alpha f \in L_p[a, b]$ for $1 \leq p < 1/\alpha$ and*

$$D_a^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \left(\frac{f(a)}{(x-a)^\alpha} + \int_a^x f'(t)(x-t)^{-\alpha} dt \right).$$

A proof of this Lemma can be found in [33, Lemma 2.11]. We now consider two examples for fractional derivatives to gain further insight into non-integer order differentiation:

Example 4.1.2 *Let $f(x) = (x-a)^c$ for some $c > -1$ and $\alpha > 0$. Then, in view of Example 4.1.1,*

$$D_a^\alpha f(x) = D^{[\alpha]} J_a^{[\alpha]-\alpha} f(x) = \frac{\Gamma(c+1)}{\Gamma([\alpha] - \alpha + c + 1)} D^{[\alpha]} (x-a)^{[\alpha]-\alpha+c}.$$

It follows that for the case, where $(-\alpha + c) \in \mathbb{N}$, the right-hand side is simply the $[\alpha]$ -th derivative of a classical polynomial of degree $([\alpha] - \alpha + c) \in \{0, 1, \dots, [\alpha] - 1\}$, and thus the expression vanishes, i.e.

$$D_a^\alpha [(\cdot - a)^{\alpha-n}](x) = 0 \text{ for all } \alpha > 0, n \in \{1, 2, \dots, [\alpha]\}.$$

On the other hand we find in the case that $(-\alpha + c) \notin \mathbb{N}$ that

$$D_a^\alpha [(\cdot - a)^c](x) = \frac{\Gamma(c+1)}{\Gamma(c+1-\alpha)} (x-a)^{c-\alpha}.$$

The two relations in this example are simple generalizations of the classical case of integer order derivatives. But nevertheless, the fractional derivative exhibits a noteworthy behaviour. From the above example we note, that the Riemann-Liouville derivative of a constant is not zero, as opposed to the integer case. Moreover, the next example will show that a fractional derivative in general cannot be derived in a direct fashion from the integer case.

Example 4.1.3 *Let $f(x) = \exp(\lambda x)$ for some $\lambda > 0$, and let $\alpha > 0$, $\alpha \notin \mathbb{N}$. Then*

$$D_a^\alpha f(x) = \frac{\exp(\lambda a)}{\Gamma(1-\alpha)} (x-a)^{-\alpha} {}_1F_1(1; 1-\alpha; \lambda(x-a)),$$

where ${}_1F_1$ denotes Kummer's confluent hypergeometric function (see (3.15)).

While this expression again coincides for integer values $\alpha = n \in \mathbb{N}$ with the classical result

$$(4.4) \quad D_a^n \exp(\lambda x) = \lambda^n \exp(\lambda x),$$

the fractional counterpart looks somewhat different. If we would have used a different definition for the fractional derivative, known as Liouville derivative ((1.3) in Chapter 1),

where the lower limit is set at minus infinity, i.e. $a = -\infty$ we would have obtained the classical result (4.4). This shows a generic dilemma one has to face when using fractional operators: There exists more than one way to generalize integer order integrals and derivatives to fractional ones and each of those has its own merits, as we will see for some definitions in the upcoming sections. For our purpose however, the Liouville operator would lead us to an analysis on unbounded intervals, which is not a natural setting for the differential equations to be considered later on.

Classical differential operators $\{D^n : n \in \mathbb{N}_0\}$ exhibit a semigroup property, which follows immediately from their definition. Furthermore, we have proven in Theorem 4.1.2 that the Riemann-Liouville integral operators also form a semigroup. The following theorem yields a similar result for the Riemann-Liouville differential operator:

Theorem 4.1.9 *Assume that $\alpha_1, \alpha_2 \geq 0$. Moreover, let $g \in L_1[a, b]$ and $f = J_a^{\alpha_1 + \alpha_2} g$. Then,*

$$D_a^{\alpha_1} D_a^{\alpha_2} f = D_a^{\alpha_1 + \alpha_2} f.$$

Proof: By our assumption on f and the definition of the Riemann-Liouville differential operator,

$$D_a^{\alpha_1} D_a^{\alpha_2} f = D_a^{\alpha_1} D_a^{\alpha_2} J_a^{\alpha_1 + \alpha_2} g = D^{[\alpha_1]} J_a^{[\alpha_1] - \alpha_1} D^{[\alpha_2]} J_a^{[\alpha_2] - \alpha_2} J_a^{\alpha_1 + \alpha_2} g.$$

The semigroup property of the integral operators allows us to rewrite this expression as

$$\begin{aligned} D_a^{\alpha_1} D_a^{\alpha_2} f &= D^{[\alpha_1]} J_a^{[\alpha_1] - \alpha_1} D^{[\alpha_2]} J_a^{[\alpha_2] + \alpha_1} g \\ &= D^{[\alpha_1]} J_a^{[\alpha_1] - \alpha_1} D^{[\alpha_2]} J_a^{[\alpha_2]} J_a^{\alpha_1} g. \end{aligned}$$

By the fact that the classical differential operator is left inverse to integer integration and the fact that the orders of the integral and differential operators involved are natural numbers the expression is equivalent to

$$D_a^{\alpha_1} D_a^{\alpha_2} f = D^{[\alpha_1]} J_a^{[\alpha_1] - \alpha_1} J_a^{\alpha_1} g = D^{[\alpha_1]} J_a^{[\alpha_1]} g$$

where we have once again used the semigroup property of fractional integration. Again applying the integer differential operator as left inverse of the integral we find that

$$D_a^{\alpha_1} D_a^{\alpha_2} f = g.$$

The proof that $D_a^{\alpha_1 + \alpha_2} f = g$ goes along similar lines. □

We only need to know the existence of a function g in Theorem 4.1.9 in order to apply the given identity. On the other hand in view of Theorem 4.1.4 the condition on f implies not only a certain degree of smoothness but also the fact, that as $x \rightarrow a$, $f(x) \rightarrow 0$ sufficiently fast. These restrictions are not a mere technicality, but they rather prove that an unconditional semigroup property of fractional differentiation does not hold. We give two examples, which show how the semigroup properties

$$(4.5) \quad D_a^{\alpha_1} D_a^{\alpha_2} f = D_a^{\alpha_1 + \alpha_2} f$$

and

$$(4.6) \quad D_a^{\alpha_1} D_a^{\alpha_2} f = D_a^{\alpha_2} D_a^{\alpha_1} f$$

are infringed, if the restrictions on f of Theorem 4.1.4 are disregarded.

Example 4.1.4 1. Let $f(x) = x^{-1/2}$ and $\alpha_1 = \alpha_2 = 1/2$. By the results of Example 4.1.2 we then have $D_0^{\alpha_1}f(x) = D_0^{\alpha_2}f(x) = 0$, and hence also $D_0^{\alpha_1}D_0^{\alpha_2}f(x) = 0$, but $D_0^{\alpha_1+\alpha_2}f(x) = D^1f(x) = -(2x^{3/2})^{-1}$ and thus property (4.5) is met while property (4.6) is violated.

2. If on the other hand $f(x) = x^{1/2}$, $\alpha_1 = 1/2$ and $\alpha_2 = 3/2$, we obtain from Example 4.1.2, that $D_0^{\alpha_1}f(x) = \sqrt{\pi}/2$ and $D_0^{\alpha_2}f(x) = 0$. This implies $D_0^{\alpha_1}D_0^{\alpha_2}f(x) = 0$ but $D_0^{\alpha_2}D_0^{\alpha_1}f(x) = -x^{-3/2}/4 = D^2f(x) = D_0^{\alpha_1+\alpha_2}f(x)$ and thus property (4.6) is met while the semigroup property (4.5) is violated.

Remark 4.1.1 As pointed out in [150], the infringement of the semigroup property is explained by the fact that a function $f(x)$ may lie in the kernel of the differential operator D_a^α with some $\alpha \in \mathbb{R}_+$. Thus $D_a^\alpha f(x)$ will be zero and any additional fractional derivative applied afterwards will be zero as well, while any other fractional derivative of $f(x)$ will not be mapped to zero.

We now state an analogue version of Theorem 4.1.5 and Corollary 4.1.6 for the Riemann-Liouville differential operators. The proofs for these differ in details from the ones for the Riemann-Liouville integral operator; we refer for those details to the proofs given in [33, Thm. 2.13 and 2.14].

Theorem 4.1.10 Let $\alpha > 0$. Assume that $(f_k)_{k=1}^\infty$ is a uniformly convergent sequence of continuous functions on $[a, b]$, and that $D_a^\alpha f_k$ exists for every k . Moreover, assume that $(D_a^\alpha f_k)_{k=1}^\infty$ converges uniformly on $[a + \varepsilon, b]$ for every $\varepsilon > 0$. Then, for every $x \in (a, b]$, we have

$$\left(\lim_{k \rightarrow \infty} D_a^\alpha f_k \right) (x) = \left(D_a^\alpha \lim_{k \rightarrow \infty} f_k \right) (x).$$

Corollary 4.1.11 Let f be analytic in $(a - h, a + h)$ for some $h > 0$, and let $\alpha > 0$, $\alpha \notin \mathbb{N}$. Then

$$D_a^\alpha f(x) = \sum_{k=0}^{\infty} \binom{\alpha}{k} \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} D^k f(x)$$

for $a < x < a + h/2$, and

$$D_a^\alpha f(x) = \sum_{k=0}^{\infty} \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} D^k f(a)$$

for $a < x < a + h$. In particular, $D_a^\alpha f$ is analytic in $(a, a + h)$.

In Chapter 2 we discussed some rules for differentiating functions that are composed from other functions in a certain way. A first generalization of those classical results to the fractional case is trivial:

Theorem 4.1.12 Let f_1 and f_2 be two functions defined on $[a, b]$ such that $D_a^\alpha f_1$ and $D_a^\alpha f_2$ exist almost everywhere. Moreover, let $c_1, c_2 \in \mathbb{R}$. Then, $D_a^\alpha (c_1 f_1 + c_2 f_2)$ exists almost everywhere, and

$$D_a^\alpha (c_1 f_1 + c_2 f_2) = c_1 D_a^\alpha f_1 + c_2 D_a^\alpha f_2.$$

Proof: This linearity property of the fractional differential operator is an immediate consequence of the definition of D_a^α . \square

A more complex result in the classical case was given by Leibniz' formula as generalized product rule. For Riemann-Liouville derivatives a similar result can be obtained:

Theorem 4.1.13 (Leibniz' formula for Riemann-Liouville operators) *Let $\alpha > 0$, and assume that f and g are analytic on $(a - h, a + h)$. Then,*

$$\begin{aligned} D_a^\alpha[f g](x) &= \sum_{k=0}^{[\alpha]} \binom{\alpha}{k} (D^k f)(x) (D_a^{\alpha-k} g)(x) \\ &\quad + \sum_{k=[\alpha]+1}^{\infty} \binom{\alpha}{k} (D^k f)(x) (J_a^{k-\alpha} g)(x) \end{aligned}$$

for $a < x < a + h/2$.

Proof: In view of Corollary 4.1.11 we have

$$D_a^\alpha[f g](x) = \sum_{k=0}^{\infty} \binom{\alpha}{k} \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} D^k[f g](x).$$

Now we apply the standard Leibniz formula to $D^k[f g]$ and interchange the order of summation. This yields

$$\begin{aligned} D_a^\alpha[f g](x) &= \sum_{k=0}^{\infty} \binom{\alpha}{k} \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} \sum_{j=0}^k \binom{k}{j} D^j f(x) D^{k-j} g(x) \\ &= \sum_{j=0}^{\infty} \sum_{k=j}^{\infty} \binom{\alpha}{k} \frac{(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} \binom{k}{j} D^j f(x) D^{k-j} g(x) \\ &= \sum_{j=0}^{\infty} D^j f(x) \sum_{\ell=0}^{\infty} \binom{\alpha}{\ell+j} \frac{(x-a)^{\ell+j-\alpha}}{\Gamma(\ell+j+1-\alpha)} \binom{\ell+j}{j} D^\ell g(x). \end{aligned}$$

The observation $\binom{\alpha}{\ell+j} \binom{\ell+j}{j} = \binom{\alpha}{j} \binom{\alpha-j}{\ell}$ gives us

$$\begin{aligned} D_a^\alpha[f g](x) &= \sum_{j=0}^{\infty} D^j f(x) \binom{\alpha}{j} \sum_{\ell=0}^{\infty} \binom{\alpha-j}{\ell} \frac{(x-a)^{\ell+j-\alpha}}{\Gamma(\ell+j+1-\alpha)} D^\ell g(x) \\ &= \sum_{j=0}^{[\alpha]} \binom{\alpha}{j} D^j f(x) \sum_{\ell=0}^{\infty} \binom{\alpha-j}{\ell} \frac{(x-a)^{\ell+j-\alpha}}{\Gamma(\ell+j+1-\alpha)} D^\ell g(x) \\ &\quad + \sum_{j=[\alpha]+1}^{\infty} \binom{\alpha}{j} D^j f(x) \sum_{\ell=0}^{\infty} \binom{\alpha-j}{\ell} \frac{(x-a)^{\ell+j-\alpha}}{\Gamma(\ell+j+1-\alpha)} D^\ell g(x). \end{aligned}$$

By the first parts of Corollaries 4.1.11 and 4.1.6, respectively, we may replace the inner sums, and the desired result follows. \square

A number of important differences between the classical and the fractional formulation of Leibniz' formula need to be addressed. We note that both functions are assumed to be analytic as requisites of Theorem 4.1.13. This requirement is obvious for the function f in order to have a meaningful right-hand side in the identity in Theorem 4.1.13, where k runs through all nonnegative integers. For g however only derivatives up to order α are needed. But in our proof we used the analyticity of the product fg , which is generally only assured if g is analytic too. As a result two important properties of the classical Leibniz rule do not transfer to the fractional case. First the fractional Leibniz' formula is not symmetric due to the second term on the right-hand side. Secondly we need to know infinitely many derivatives of the function f in order to calculate the derivatives of the product fg , while in the classical case only derivative of order $0, 1, \dots, n$ are needed. Nevertheless, we recover the classical Leibniz' formula by choosing $\alpha \in \mathbb{N}$ because then all binomial coefficients of the second sum are zero.

Another important rule for the classical case was the chain rule. While there exists a formulation of a fractional chain rule [122, §2.7.3], its structure is so complex that a practical use is unlikely.

Having defined both, the Riemann-Liouville integral and the differential operator, we can now state results on the interaction of both. A first result is concerned with the inverse property of the two operators:

Theorem 4.1.14 *Let $\alpha > 0$. Then, for every $f \in L_1[a, b]$,*

$$D_a^\alpha J_a^\alpha f = f$$

almost everywhere. If furthermore there exists a function $g \in L_1[a, b]$ such that $f = J_a^\alpha g$ then

$$J_a^\alpha D_a^\alpha f = f$$

almost everywhere.

Proof: For the first statement we proceed as in the proof of Theorem 4.1.9: Let $n = \lceil \alpha \rceil$. Then, by the definition of D_a^α and the semigroup property of fractional integration and the left inverse of the classical differential operator,

$$D_a^\alpha J_a^\alpha f(x) = D^n J_a^{n-\alpha} J_a^\alpha f(x) = D^n J_a^n f(x) = f(x).$$

The second statement is an immediate consequence of the previous result: We have, by definition of f and Theorem 4.1.14, that

$$J_a^\alpha D_a^\alpha f = J_a^\alpha [D_a^\alpha J_a^\alpha g] = J_a^\alpha g = f.$$

□

We thus have shown by the first statement, that the Riemann-Liouville differential operator is indeed left-inverse to the Riemann-Liouville integral operator, while we can only obtain a right-inverse under the condition $f = J_a^\alpha g$, which is similar to the classical case. If f does not satisfy this condition, a different representation for $J_a^\alpha D_a^\alpha f$ can be given, as proven in [33, Thm. 2.20].

Theorem 4.1.15 Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Assume that f is such that $J_a^{n-\alpha} f \in A^n[a, b]$. Then,

$$J_a^\alpha D_a^\alpha f(x) = f(x) - \sum_{k=0}^{n-1} \frac{(x-a)^{\alpha-k-1}}{\Gamma(\alpha-k)} \lim_{z \rightarrow a+} D^{n-k-1} J_a^{n-\alpha} f(z).$$

Specifically, for $0 < \alpha < 1$ we have

$$J_a^\alpha D_a^\alpha f(x) = f(x) - \frac{(x-a)^{\alpha-1}}{\Gamma(\alpha)} \lim_{z \rightarrow a+} J_a^{1-\alpha} f(z).$$

With the result of this theorem we can prove the fractional version of the classical Taylor expansion, given in Theorem 2.1.10:

Theorem 4.1.16 (Fractional Taylor expansion) Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Assume that f is such that $J_a^{n-\alpha} f \in A^n[a, b]$. Then

$$\begin{aligned} f(x) &= \frac{(x-a)^{\alpha-n}}{\Gamma(\alpha-n+1)} \lim_{z \rightarrow a+} J_a^{n-\alpha} f(z) \\ &+ \sum_{k=1}^{n-1} \frac{(x-a)^{k+\alpha-n}}{\Gamma(k+\alpha-n+1)} \lim_{z \rightarrow a+} D_a^{k+\alpha-n} f(z) + J_a^\alpha D_a^\alpha f(x). \end{aligned}$$

Proof: By change of variables we obtain from Theorem 4.1.15 the equality

$$f(x) = \sum_{k=0}^{n-1} \frac{(x-a)^{k+\alpha-n}}{\Gamma(k+\alpha-n+1)} \lim_{z \rightarrow a+} D_a^k J_a^{n-\alpha} f(z) + J_a^\alpha D_a^\alpha f(x).$$

We now move the summand for $k = 0$ out of the sum; for the remaining terms we apply Lemma 4.1.7. This gives the result. \square

Before we consider (partial) differential equations utilizing the Riemann-Liouville differential operator, we consider a number of different fractional integral and differential operators, which were already mentioned in the historical review in Chapter 1 and will become of great interest in later chapters.

4.1.2 Caputo operator

In 1967 a paper [20] by M. Caputo was published, where a new definition of a fractional derivative was used. In this section we state the definition and some properties of this new operator, today called *Caputo fractional derivative* and most importantly show its connection to the fractional Riemann-Liouville integral and differential operators. We begin with a formal definition:

Definition 4.1.3 Let $\alpha \in \mathbb{R}_+$ and $n = \lceil \alpha \rceil$. The operator D_{*a}^α , defined by

$$(4.7) \quad D_{*a}^\alpha f(x) = J_a^{n-\alpha} D^n f(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-t)^{n-\alpha-1} \left(\frac{d}{dt} \right)^n f(t) dt$$

for $a \leq x \leq b$, is called the Caputo differential operator of order α .

We note that the definition of the Caputo differential operator also utilizes the Riemann-Liouville integral operator, but compared with the Riemann-Liouville derivative the sequence, in which integer order differentiation and fractional integration are applied, is interchanged. This fact has a rather important impact on the structure of the fractional derivatives, which becomes obvious by the following example:

Example 4.1.5 Let $\alpha \geq 0$, $n = \lceil \alpha \rceil$ and $f(x) = (x - a)^c$ for some $c \geq 0$. Then,

$$D_{*a}^\alpha f(x) = \begin{cases} 0 & \text{if } c \in \{0, 1, 2, \dots, n-1\}, \\ \frac{\Gamma(c+1)}{\Gamma(c+1-\alpha)}(x-a)^{c-\alpha} & \text{if } c \in \mathbb{N} \text{ and } c \geq n \\ & \text{or } c \notin \mathbb{N} \text{ and } c > n-1. \end{cases}$$

If we compare this result with the one in Example 4.1.2, where we applied the Riemann-Liouville differential operator on the function f , we notice in particular that the two operators have different kernels, and that the domains of the two operators (exhibited here in terms of the allowed range of the parameter c) are also different. However, a first result on the Caputo differential operator states an important connection between the two fractional derivatives.

Theorem 4.1.17 Let $\alpha \geq 0$ and $n = \lceil \alpha \rceil$. Moreover, assume that $D_a^\alpha f$ exists and f possesses $(n-1)$ derivatives at a . Then,

$$D_{*a}^\alpha f = D_a^\alpha [f - T_{n-1}[f; a]]$$

almost everywhere, where $T_{n-1}[f; a]$ denotes the Taylor polynomial of degree $n-1$ for the function f , centered at a (see Definition 2.1.4).

Proof: By Lemma 4.1.7 and Definition 4.1.1 we have

$$\begin{aligned} (4.8) \quad D_a^\alpha [f - T_{n-1}[f; a]](x) &= D^n J_a^{n-\alpha} [f - T_{n-1}[f; a]](x) \\ &= \frac{d^n}{dx^n} \int_a^x \frac{(x-t)^{n-\alpha-1}}{\Gamma(n-\alpha)} (f(t) - T_{n-1}[f; a](t)) dt. \end{aligned}$$

A partial integration of the integral is permitted and yields

$$\begin{aligned} &\int_a^x \frac{1}{\Gamma(n-\alpha)} (f(t) - T_{n-1}[f; a](t)) (x-t)^{n-\alpha-1} dt \\ &= -\frac{1}{\Gamma(n-\alpha+1)} [(f(t) - T_{n-1}[f; a](t)) (x-t)^{n-\alpha}]_{t=a}^{t=x} \\ &\quad + \frac{1}{\Gamma(n-\alpha+1)} \int_a^x (Df(t) - DT_{n-1}[f; a](t)) (x-t)^{n-\alpha} dt. \end{aligned}$$

The term outside the integral is zero (the first factor vanishes at the lower bound, the second vanishes at the upper bound). Thus,

$$J_a^{n-\alpha} [f - T_{n-1}[f; a]] = J_a^{n-\alpha+1} D[f - T_{n-1}[f; a]].$$

Under our assumptions, we may repeat this process a total number of n times, which results in

$$\begin{aligned} J_a^{n-\alpha}[f - T_{n-1}[f; a]] &= J_a^{2n-\alpha}D^n[f - T_{n-1}[f; a]] \\ &= J_a^n J_a^{n-\alpha}D^n[f - T_{n-1}[f; a]]. \end{aligned}$$

We note that $D^n T_{n-1}[f; a] \equiv 0$ because $T_{n-1}[f; a]$ is a polynomial of degree $n - 1$. Thus, the last identity can be simplified to

$$J_a^{n-\alpha}[f - T_{n-1}[f; a]] = J_a^n J_a^{n-\alpha}D^n f.$$

This may be combined with (4.8) to obtain

$$D_a^\alpha[f - T_{n-1}[f; a]](x) = D^n J_a^n J_a^{n-\alpha}D^n f = J_a^{n-\alpha}D^n f = D_{*a}^\alpha f.$$

□

We note that this theorem states, that the Caputo derivative of a function f is only defined if the Riemann-Liouville derivative of f exists and additionally f is $(n - 1)$ times differentiable in the classical sense to ensure the existence of the Taylor polynomial. Another way to express the relation between both fractional differential operators is given by the following lemma:

Lemma 4.1.18 *Let $\alpha \geq 0$ and $n = \lceil \alpha \rceil$. Assume that f is such that both $D_{*a}^\alpha f$ and $D_a^\alpha f$ exist. Then,*

$$D_{*a}^\alpha f(x) = D_a^\alpha f(x) - \sum_{k=0}^{n-1} \frac{D^k f(a)}{\Gamma(k - \alpha + 1)} (x - a)^{k-\alpha}.$$

Proof: In view of the definition of the Caputo derivative and Example 4.1.2,

$$\begin{aligned} D_{*a}^\alpha f(x) &= D_a^\alpha f(x) - \sum_{k=0}^{n-1} \frac{D^k f(a)}{k!} D_a^\alpha [(\cdot - a)^k](x) \\ &= D_a^\alpha f(x) - \sum_{k=0}^{n-1} \frac{D^k f(a)}{\Gamma(k - \alpha + 1)} (x - a)^{k-\alpha}. \end{aligned}$$

□

An immediate consequence of this Lemma is

Lemma 4.1.19 *Let $\alpha \geq 0$ and $n = \lceil \alpha \rceil$. Assume that f is such that both $D_{*a}^\alpha f$ and $D_a^\alpha f$ exist. Moreover, let $D^k f(a) = 0$ for $k = 0, 1, \dots, n - 1$ (i.e. we assume f to have an n -fold zero at a). Then,*

$$D_a^\alpha f = D_{*a}^\alpha f.$$

This is especially important in view of differential equations of fractional order. It basically states, that those equations formulated with Riemann-Liouville derivatives coincide with those formulated with Caputo derivatives, if the initial condition(s) are homogeneous. We will come back to this fact in Chapter 4.2.

Considering the interaction of Riemann-Liouville integrals and Caputo differential operators, we find that the Caputo derivative is also a left inverse of the Riemann-Liouville integral:

Theorem 4.1.20 *If f is continuous and $\alpha \geq 0$, then*

$$D_{*a}^\alpha J_a^\alpha f = f.$$

Proof: Let $g = J_a^\alpha f$. By Theorem 4.1.3, we have $D^k g(a) = 0$ for $k = 0, 1, \dots, n-1$, and thus (in view of Lemma 4.1.19 and Theorem 4.1.14)

$$D_{*a}^\alpha J_a^\alpha f = D_{*a}^\alpha g = D_a^\alpha g = D_a^\alpha J_a^\alpha f = f.$$

□

Additionally, the Caputo derivative also is not the right inverse of the Riemann-Liouville integral [33, see Thm. 3.5]:

Theorem 4.1.21 *Assume that $\alpha \geq 0$, $n = \lceil \alpha \rceil$, and $f \in A^n[a, b]$. Then*

$$J_a^\alpha D_{*a}^\alpha f(x) = f(x) - \sum_{k=0}^{n-1} \frac{D^k f(a)}{k!} (x-a)^k.$$

With this result we can immediately state a fractional analogue of Taylor's theorem for Caputo derivatives:

Corollary 4.1.22 (Taylor expansion for Caputo derivatives) *Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Assume that f is such that $f \in A^n[a, b]$. Then*

$$f(x) = \sum_{k=0}^{n-1} \frac{D^k f(a)}{k!} (x-a)^k + J_a^\alpha D_{*a}^\alpha f(x).$$

A comparison of this result with Taylor's expansion in case of Riemann-Liouville differential operators given in Theorem 4.1.16 will - apart from the simpler structure in the Caputo case - give a decisive difference concerning differential equations, which we will discuss in detail in Chapter 4.2.

In terms of derivation rules for the Caputo derivative of composed functions, we can find similar, but not identical, results to those for the Riemann-Liouville derivative. We start with the linearity.

Theorem 4.1.23 *Let f_1 and f_2 be two functions defined on $[a, b]$ such that $D_{*a}^\alpha f_1$ and $D_{*a}^\alpha f_2$ exist almost everywhere. Moreover, let $c_1, c_2 \in \mathbb{R}$. Then, $D_{*a}^\alpha (c_1 f_1 + c_2 f_2)$ exists almost everywhere, and*

$$D_{*a}^\alpha (c_1 f_1 + c_2 f_2) = c_1 D_{*a}^\alpha f_1 + c_2 D_{*a}^\alpha f_2.$$

Proof: This linearity property of the fractional differential operator is an immediate consequence of the definition of D_{*a}^α . □

For the formula of Leibniz, we only state the case $0 < \alpha < 1$ explicitly.

Theorem 4.1.24 (Leibniz' formula for Caputo operators) *Let $0 < \alpha < 1$, and assume that f and g are analytic on $(a - h, a + h)$. Then,*

$$\begin{aligned} D_{*a}^\alpha[f g](x) &= \frac{(x-a)^{-\alpha}}{\Gamma(1-\alpha)} g(a)(f(x) - f(a)) + (D_{*a}^\alpha g(x)) f(x) \\ &\quad + \sum_{k=1}^{\infty} \binom{\alpha}{k} (J_a^{k-\alpha} g(x)) D_{*a}^k f(x). \end{aligned}$$

Proof: We apply the definition of the Caputo derivative and find

$$D_{*a}^\alpha[f g] = D_a^\alpha[f g - f(a)g(a)] = D_a^\alpha[f g] - f(a)g(a)D_a^\alpha[1].$$

Next we use Leibniz' formula for Riemann-Liouville derivatives and find

$$D_{*a}^\alpha[f g] = f(D_a^\alpha g) + \sum_{k=1}^{\infty} \binom{\alpha}{k} (D_a^k f)(J_a^{k-\alpha} g) - f(a)g(a)D_a^\alpha[1].$$

Now we add and subtract $f(a)g(a)(D_a^\alpha[1])$ and rearrange to obtain

$$\begin{aligned} D_{*a}^\alpha[f g] &= f(D_a^\alpha[g - g(a)]) + \sum_{k=1}^{\infty} \binom{\alpha}{k} (D_a^k f)(J_a^{k-\alpha} g) \\ &\quad + g(a)(f - f(a))D_a^\alpha[1] \\ &= f(D_{*a}^\alpha g) + \sum_{k=1}^{\infty} \binom{\alpha}{k} (D_{*a}^k f)(J_a^{k-\alpha} g) + g(a)(f - f(a))D_a^\alpha[1], \end{aligned}$$

where we have used the fact that, for $k \in \mathbb{N}$, $D_a^k = D^k = D_{*a}^k$. Finally we introduce the explicit expression for $D_a^\alpha[1]$ from Example 4.1.2 to complete the proof. \square

The next two results on the Caputo differential operator establish another significant difference between Riemann-Liouville and Caputo derivatives.

Lemma 4.1.25 *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Moreover, assume that $f \in C^n[a, b]$. Then, $D_{*a}^\alpha f$ is continuous on $[a, b]$ and $D_{*a}^\alpha f(a) = 0$.*

Proof: By definition and Theorem 4.1.17, $D_{*a}^\alpha f = J_a^{n-\alpha} D^n f$. The result follows from Theorem 4.1.3 because $D^n f$ is assumed to be continuous. \square

We may relax the conditions on f slightly to obtain the following result:

Lemma 4.1.26 *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Moreover, let that $f \in A^n[a, b]$ and assume that $D_{*a}^{\hat{\alpha}} f \in C[a, b]$ for some $\hat{\alpha} \in (\alpha, n)$. Then, $D_{*a}^\alpha f$ is continuous on $[a, b]$ and $D_{*a}^\alpha f(a) = 0$.*

Proof: By definition, Theorem 4.1.17 and the semigroup property of fractional integration,

$$D_{*a}^\alpha f = J_a^{n-\alpha} D^n f = J_a^{\hat{\alpha}-\alpha} J_a^{n-\hat{\alpha}} D^n f = J_a^{\hat{\alpha}-\alpha} D_{*a}^{\hat{\alpha}} f.$$

Thus the claim follows by virtue of Theorem 4.1.3. \square

A comparison with, e.g., Example 4.1.2 for $f(x) = 1$ and $\alpha > 0$, $\alpha \notin \mathbb{N}$, reveals that we are not allowed to replace D_{*a}^α by D_a^α here.

4.1.3 Grünwald-Letnikov operator

Nearly simultaneous with the development of the Riemann-Liouville definition of fractional integration and differentiation another definition for a non-integer derivative was developed independently by Grünwald and Letnikov. Their definition will allow us later on to construct numerical methods for differential equations of fractional order, described with either Riemann-Liouville or Caputo derivatives. We start with a formal definition.

Definition 4.1.4 Let $\alpha \in \mathbb{R}_+$. The operator ${}^{GL}D_a^\alpha$, defined by

$$(4.9) \quad {}^{GL}D_a^\alpha f(x) = \lim_{\substack{h \rightarrow 0 \\ mh = x-a}} \frac{(\Delta_h^\alpha f)(x)}{h^\alpha} = \lim_{\substack{h \rightarrow 0 \\ mh = x-a}} \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} f(x - kh), \quad \alpha > 0,$$

for $a \leq x \leq b$, is called the Grünwald-Letnikov fractional derivative of order α .

In this definition the term $(\Delta_h^\alpha f)(x)$ is a fractional formulation of a backward difference. The definition holds for arbitrary functions $f(x)$, but the convergence of the infinite sum cannot be ensured for all functions. However, if the Grünwald-Letnikov differential operator is used in fractional order differential equations, we may set the solution $y(x)$ formally to 0 for the negative real axis. As a result the infinite sum in Definition 4.1.4 collapses to a finite sum in these cases. It is also possible to define a *Grünwald-Letnikov fractional integral of order α* by replacing α in (4.9) with $-\alpha$, i.e.

$${}^{GL}J_a^\alpha f(x) = \lim_{\substack{h \rightarrow 0 \\ mh = x-a}} h^\alpha \sum_{k=0}^m (-1)^k \binom{-\alpha}{k} f(x - kh) = \lim_{\substack{h \rightarrow 0 \\ mh = x-a}} \frac{h^\alpha}{\Gamma(\alpha)} \sum_{k=0}^m \frac{\Gamma(k+\alpha)}{\Gamma(k+1)} f(x - kh), \quad \alpha > 0.$$

However, for our purpose the derivative is far more important.

In the next theorem we state an important result, which will give us an insight in the connection between the Grünwald-Letnikov derivative and the two earlier defined fractional derivatives, namely the Riemann-Liouville and the Caputo derivative.

Theorem 4.1.27 Let $\alpha \geq 0$, $n = \lceil \alpha \rceil$ and $f \in C^n[a, b]$, then

$$(4.10) \quad {}^{GL}D_a^\alpha f(x) = \sum_{k=0}^{n-1} \frac{f^{(k)}(a)(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} + \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-t)^{n-1-\alpha} f^{(n)}(t) dt.$$

Before we can prove this theorem we need a result, first stated by A. V. Letnikov in [81]:

Theorem 4.1.28 Let $(b_k)_{k=1}^\infty$ and $(a_{n,k})_{n,k=1}^\infty$ be given sequences, which satisfy

$$(4.11) \quad \lim_{k \rightarrow \infty} b_k = 1,$$

$$(4.12) \quad \lim_{n \rightarrow \infty} a_{n,k} = 0, \quad \text{for all } k,$$

$$(4.13) \quad \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} = A,$$

$$(4.14) \quad \sum_{k=1}^n |a_{n,k}| < K, \quad \text{for all } n,$$

with some numbers $A, K \in \mathbb{R}$. Then

$$(4.15) \quad \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} b_k = A.$$

Proof: In order to prove this statement we first note that by condition (4.12) for every fixed r

$$\lim_{n \rightarrow \infty} \sum_{k=1}^{r-1} a_{n,k} b_k = 0 \quad \text{and} \quad \lim_{n \rightarrow \infty} \sum_{k=1}^{r-1} a_{n,k} = 0$$

holds. Additionally it follows from condition (4.11), that

$$(4.16) \quad b_k = 1 - c_k, \quad \text{where} \quad \lim_{k \rightarrow \infty} c_k = 0.$$

We thus obtain

$$\begin{aligned} \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} b_k &= \lim_{n \rightarrow \infty} \sum_{k=r}^n a_{n,k} b_k \\ &= \lim_{n \rightarrow \infty} \sum_{k=r}^n a_{n,k} - \lim_{n \rightarrow \infty} \sum_{k=r}^n a_{n,k} c_k \\ &= \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} - \lim_{n \rightarrow \infty} \sum_{k=r}^n a_{n,k} c_k \\ &= A - \lim_{n \rightarrow \infty} \sum_{k=r}^n a_{n,k} c_k \end{aligned}$$

given that the limits exist. With this result we can perform the following estimation:

$$\begin{aligned} \left| A - \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} b_k \right| &< \lim_{n \rightarrow \infty} \sum_{k=r}^n |a_{n,k}| |c_k| \\ &< c^* \lim_{n \rightarrow \infty} \sum_{k=r}^n |a_{n,k}| \leq c^* \lim_{n \rightarrow \infty} \sum_{k=1}^n |a_{n,k}| \\ &< c^* K, \end{aligned}$$

where $c^* = \max_{k \geq r} |c_k|$. By (4.16) it follows that for any arbitrarily small $\varepsilon > 0$, there exists a variable r such that $c^* < \varepsilon/K$ and thus

$$\left| A - \lim_{n \rightarrow \infty} \sum_{k=1}^n a_{n,k} b_k \right| < \varepsilon,$$

which means that (4.15) holds. □

Proof: (of Theorem 4.1.27) At first we note, that the well known property of the binomial coefficient

$$(4.17) \quad \binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1}, \quad k, n \in \mathbb{N}$$

transfers to the generalized binomial coefficient, where $\alpha \in \mathbb{R}$. This identity can be proven by simple calculations using

$$\binom{\alpha}{k} = \frac{\Gamma(k - \alpha)}{\Gamma(-\alpha)\Gamma(k + 1)}.$$

Denoting the right-hand side of (4.9) without the limit as $f_h^\alpha(x)$ we can write

$$\begin{aligned} f_h^\alpha(x) &= \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} f(x - kh) \\ &= \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha-1}{k} f(x - kh) + \frac{1}{h^\alpha} \sum_{k=1}^m (-1)^k \binom{\alpha-1}{k-1} f(x - kh) \\ &= \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha-1}{k} f(x - kh) + \frac{1}{h^\alpha} \sum_{k=0}^{m-1} (-1)^{k+1} \binom{\alpha-1}{k} f(x - (k+1)h) \\ &= \frac{1}{h^\alpha} (-1)^m \binom{\alpha-1}{m} f(a) + \frac{1}{h^\alpha} \sum_{k=0}^{m-1} (-1)^k \binom{\alpha-1}{k} (f(x - kh) - f(x - (k+1)h)) \end{aligned}$$

Let us denote by $\Delta f(x - kh) := f(x - kh) - f(x - (k+1)h)$ the classical first backward difference at the point $x + kh$ and by $\nabla f(a) := f(a + h) - f(a)$ the classical first forward difference at the point a . Furthermore, we use the classical notation Δ^k and ∇^k to denote higher order backward and forward differences respectively and set $\Delta^0 f(x) = f(x) = \nabla^0 f(x)$. If we apply property (4.17) again we get

$$\begin{aligned} f_h^\alpha(x) &= \frac{1}{h^\alpha} (-1)^m \binom{\alpha-1}{m} \nabla^0 f(a) + \frac{1}{h^\alpha} (-1)^{m-1} \binom{\alpha-2}{m-1} \nabla f(a) \\ &\quad + \frac{1}{h^\alpha} \sum_{k=0}^{m-2} (-1)^k \binom{\alpha-2}{k} \Delta^2 f(x - kh) \end{aligned}$$

and after applying the same method n times we obtain

$$\begin{aligned} (4.18) \quad f_h^\alpha(x) &= \frac{1}{h^\alpha} \sum_{k=0}^{n-1} (-1)^{m-k} \binom{\alpha-k-1}{m-k} \nabla^k f(a) \\ &\quad + \frac{1}{h^\alpha} \sum_{k=0}^{m-n} (-1)^k \binom{\alpha-n}{k} \Delta^n f(x - kh). \end{aligned}$$

We now only consider the k -th term in the first sum

$$\begin{aligned} &\frac{1}{h^\alpha} (-1)^{m-k} \binom{\alpha-k-1}{m-k} \nabla^k f(a) \\ &= \left(\frac{m-k}{mh} \frac{m}{m-k} \right)^{\alpha-k} \frac{1}{h^k} (-1)^{m-k} \binom{\alpha-k-1}{m-k} \nabla^k f(a) \\ &= \left(\frac{m-k}{b-a} \right)^{\alpha-k} \left(\frac{m}{m-k} \right)^{\alpha-k} (-1)^{m-k} \binom{\alpha-k-1}{m-k} \frac{\nabla^k f(a)}{h^k}, \end{aligned}$$

and evaluate the limit of this term as $h \rightarrow 0$ (or $m \rightarrow \infty$), which yields

$$\begin{aligned} & \lim_{m \rightarrow \infty} \frac{1}{h^\alpha} (-1)^{m-k} \binom{\alpha - k - 1}{m - k} \nabla^k f(a) \\ &= (b - a)^{-\alpha+k} \lim_{m \rightarrow \infty} (-1)^{m-k} \binom{\alpha - k - 1}{m - k} (m - k)^{\alpha-k} \\ & \quad \times \lim_{m \rightarrow \infty} \left(\frac{m}{m - k} \right)^{\alpha-k} \lim_{h \rightarrow 0} \frac{\nabla^k f(a)}{h^k}, \end{aligned}$$

given that the stated limits exist. For the existence we note that

$$\begin{aligned} & \lim_{m \rightarrow \infty} (-1)^{m-k} \binom{\alpha - k - 1}{m - k} (m - k)^{\alpha-k} \\ &= \lim_{m \rightarrow \infty} \frac{(-\alpha + k + 1)(-\alpha + k + 2) \dots (-\alpha + m)}{(m - k)^{-\alpha+k} (m - k)!} = \frac{1}{\Gamma(-\alpha + k + 1)}, \end{aligned}$$

and

$$\lim_{m \rightarrow \infty} \left(\frac{m}{m - k} \right)^{\alpha-k} = 1,$$

and finally

$$\lim_{h \rightarrow 0} \frac{\nabla^k f(a)}{h^k} = f^{(k)}(a),$$

such that the result for the limit of the k -th term of the first sum in (4.18) is given by:

$$(4.19) \quad \lim_{m \rightarrow \infty} \frac{1}{h^\alpha} (-1)^{m-k} \binom{\alpha - k - 1}{m - k} \nabla^k f(a) = \frac{f^{(k)}(a)(b - a)^{-\alpha+k}}{\Gamma(-\alpha + k + 1)}.$$

Having established the special case for the k -th term in the first sum in (4.18), we can easily state the limit of the whole sum. In order to evaluate the limit of the second sum in (4.18), we first rewrite it:

$$\begin{aligned} (4.20) \quad & \frac{1}{h^\alpha} \sum_{k=0}^{m-n} (-1)^k \binom{\alpha - n}{k} \Delta^n f(x - kh) \\ &= \frac{1}{\Gamma(-\alpha + n)} \sum_{k=0}^{m-n} (-1)^k \Gamma(-\alpha + n) \binom{\alpha - n}{k} k^{-n+1+\alpha} \\ & \quad \times h(kh)^{n-1-\alpha} \frac{\Delta^n f(x - kh)}{h^n}, \end{aligned}$$

and set

$$\begin{aligned} b_k &= (-1)^k \Gamma(-\alpha + n) \binom{\alpha - n}{k} k^{-n+1+\alpha}, \\ a_{m,k} &= h(kh)^{n-1-\alpha} \frac{\Delta^n f(x - kh)}{h^n}, \quad h = \frac{b - a}{m}. \end{aligned}$$

To apply Theorem 4.1.28 we note that

$$\lim_{k \rightarrow \infty} b_k = (-1)^k \Gamma(-\alpha + n) \binom{\alpha - n}{k} k^{-n+1+\alpha} = 1$$

and, if $n - 1 - \alpha > -1$,

$$\begin{aligned} \lim_{m \rightarrow \infty} \sum_{k=0}^{m-n} a_{m,k} &= \lim_{\substack{h \rightarrow 0 \\ mh=b-a}} \sum_{k=0}^{m-n} h(kh)^{n-1-\alpha} \frac{\Delta^n f(x - kh)}{h^n} \\ &= \int_a^x (x-t)^{n-1-\alpha} f^{(n)}(t) dt. \end{aligned}$$

Thus, after applying Theorem 4.1.28, the limit of the second sum in (4.18) is given by

$$\begin{aligned} \lim_{m \rightarrow \infty} \frac{1}{h^\alpha} \sum_{k=0}^{m-n} (-1)^k \binom{\alpha - n}{k} \Delta^n f(x - kh) \\ = \frac{1}{\Gamma(-\alpha + n)} \int_a^x (x-t)^{n-1-\alpha} f^{(n)}(t) dt. \end{aligned}$$

Finally, combining the results (4.19) and (4.21) we obtain

$$\begin{aligned} {}^{GL}D_a^\alpha f(x) &= \sum_{k=0}^{n-1} \frac{f^{(k)}(a)(x-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} \\ &\quad + \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-t)^{n-1-\alpha} f^{(n)}(t) dt. \end{aligned}$$

□

With Theorem 4.1.27 we can now easily connect the three fractional derivatives D_a^α , D_{a*}^α and ${}^{GL}D_a^\alpha$.

Corollary 4.1.29 *Let $\alpha \geq 0$, $[\alpha] = n$ and $f \in C^n[a, b]$. Then*

$${}^{GL}D_a^\alpha f(x) = T_{n-1}[f; a](x) + D_{a*}^\alpha f(x) = D_a^\alpha f(x).$$

Proof: The statement ${}^{GL}D_a^\alpha f(x) = T_{n-1}[f; a](x) + D_{a*}^\alpha f(x)$ is a direct consequence of Theorem 4.1.27 and $T_{n-1}[f; a](x) + D_{a*}^\alpha f(x) = D_a^\alpha f(x)$ has been proven in Theorem 4.1.17. □

While from a pure mathematical point of view the restriction $f \in C^n[a, b]$ narrows the class of functions, for which the connection in Corollary 4.1.29 can be established, it is rather important for applications. In addition, the definition of the Caputo operator already demands the existence of the n th derivative of the function f and thus the restriction $f \in C^n[a, b]$ is not much stronger.

For the later to be developed numerical algorithms, it is of interest to know what happens, if we only use a finite sum, i.e. $N \in \mathbb{N}$, in the definition of the Grünwald Letnikov fractional derivative.

Theorem 4.1.30 *Let $f \in C^n[0, X]$, $\alpha \geq 0$, $\lceil \alpha \rceil = n$, and $X/h = m \in \mathbb{N}$. Then the finite Grünwald-Letnikov differential operator centered at 0*

$$(4.21) \quad {}_F^{\text{GL}}D^\alpha f(x) = \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} f(x - kh)$$

yields a first order approximation for the Riemann-Liouville differential operator D^α if and only if $f(0) = 0$, i.e

$${}_F^{\text{GL}}D^\alpha f(x) = D^\alpha f(x) + \mathcal{O}(h).$$

In the case $f(0) = x_0 \neq 0$ we get an additional error term with magnitude of x_0 , i.e

$${}_F^{\text{GL}}D^\alpha f(x) = D^\alpha f(x) + \mathcal{O}(h) + \mathcal{O}(x_0).$$

Proof: This theorem will follow immediately from Corollary 4.3.14 and thus gets deferred for now. \square

As mentioned in the historical outline in Chapter 1 there are more ways to define fractional derivatives. However, for our purpose to describe numerical methods for fractional differential equations based on models of real applications, the three stated versions will be sufficient. Analytical background on different fractional operators can be found in several books on fractional calculus, e.g. [105, 110, 122, 141].

4.2 Fractional differential equations

In this part of the text we will discuss existence and uniqueness properties of ordinary differential equations involving fractional derivatives. We restrict ourselves to initial value problems (Cauchy problems) and furthermore we assume without loss of generality that the fractional derivatives are developed at the point 0. As a consequence we use from now on D^α , D_*^α and ${}^{\text{GL}}D^\alpha$ as symbols for the Riemann-Liouville, the Caputo and the Grünwald-Letnikov fractional derivatives developed at the point 0. We start our discussion with a formal definition of a fractional differential equation (FDE):

Definition 4.2.1 *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$, $n = \lceil \alpha \rceil$ and $f : A \subseteq \mathbb{R}^2 \rightarrow \mathbb{R}$. Then*

$$(4.22) \quad D^\alpha y(x) = f(x, y(x))$$

is called fractional differential equation of Riemann-Liouville type. As initial conditions for this type of FDE we use

$$(4.23) \quad D^{\alpha-k} y(0) = b_k \quad (k = 1, 2, \dots, n-1), \quad \lim_{z \rightarrow 0+} J^{n-\alpha} y(z) = b_n.$$

Similarly

$$(4.24) \quad D_*^\alpha y(x) = f(x, y(x))$$

is called fractional differential equation of Caputo type and in this case use as initial conditions

$$(4.25) \quad D^k y(0) = b_k, \quad (k = 0, 1, \dots, n-1).$$

The use of different types of initial conditions for the fractional differential equations (4.22) and (4.24) has already been mentioned in the previous chapter. They basically ensure the uniqueness of a solution of the corresponding FDE, which we will prove in the following theorems. We start with the Riemann-Liouville type.

Theorem 4.2.1 *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Moreover, let $K > 0$, $h^* > 0$, and $b_1, \dots, b_m \in \mathbb{R}$. Define*

$$G := \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq h^*, y \in \mathbb{R} \text{ for } x = 0 \text{ and} \\ |x^{n-\alpha}y - \sum_{k=1}^n b_k x^{n-k} / \Gamma(\alpha - k + 1)| < K \text{ else}\},$$

and assume that the function $f : G \rightarrow \mathbb{R}$ is continuous and bounded in G and that it fulfills a Lipschitz condition with respect to the second variable, i.e. there exists a constant $L > 0$ such that, for all (x, y_1) and $(x, y_2) \in G$, we have

$$|f(x, y_1) - f(x, y_2)| < L|y_1 - y_2|.$$

Then the fractional differential equation of Riemann-Liouville type (4.22) equipped with the initial conditions (4.23) has got a uniquely defined continuous solution $y \in C(0, h]$ where $h := \min\{h^, \tilde{h}, (\Gamma(\alpha + 1)K/M)^{1/n}\}$ with $M := \sup_{(x,z) \in G} |f(x, z)|$ and \tilde{h} being an arbitrary positive number satisfying the constraint*

$$\tilde{h} < \frac{\Gamma(2\alpha - n + 1)}{(\Gamma(\alpha - n + 1)L)^{1/\alpha}}.$$

For the fractional differential equation of Caputo type we can obtain a similar result:

Theorem 4.2.2 *Let $\alpha > 0$, $n \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. Moreover, let $K > 0$, $h^* > 0$, and $b_0, \dots, b_{n-1} \in \mathbb{R}$. Define*

$$G := [0, h^*] \times [b_0 - K, b_0 + K],$$

and let the function $f : G \rightarrow \mathbb{R}$ be continuous. Then, there exists some $h > 0$ and a function $y \in C[0, h]$ solving the fractional differential equation of Caputo type (4.24) equipped with initial conditions (4.25). For the case $\alpha \in (0, 1)$ the parameter h is given by

$$h := \min\{h^*, (K\Gamma(\alpha + 1)/M)^{1/\alpha}\}, \quad \text{with} \quad M := \sup_{(x,z) \in G} |f(x, z)|.$$

If furthermore f fulfils a Lipschitz condition with respect to the second variable, i.e.

$$|f(x, y_1) - f(x, y_2)| \leq L|y_1 - y_2|$$

with some constant $L > 0$ independent of x , y_1 , and y_2 , the function $y \in C[0, h]$ is unique.

These results are very similar to their counterparts in the classical case of first-order equations. They are even proven in a similar way. In particular, this means that we will not prove these theorems directly, but rather show that both types of fractional differential equations can be formulated as integral equations (see also the Tautochrone excursus in Chapter 1), namely Volterra integral equations:

Theorem 4.2.3 1. Under the assumptions of Theorem 4.2.1 the function $y \in C(0, h]$ is a solution to the fractional differential equation of Riemann-Liouville type (4.22), equipped with the initial conditions (4.23), if and only if it is a solution of the Volterra integral equation of the second kind

$$(4.26) \quad y(x) = \sum_{k=1}^n \frac{b_k x^{\alpha-k}}{\Gamma(\alpha-k+1)} + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

2. Under the assumptions of Theorem 4.2.2 the function $y \in C[0, h]$ is a solution to the fractional differential equation of Caputo type (4.24), equipped with the initial conditions (4.25), if and only if it is a solution of the Volterra integral equation of the second kind

$$(4.27) \quad y(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} b_k + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

Before we are going to prove these theorems, there are some noteworthy remarks with respect to the different types of fractional differential equations:

Remark 4.2.1 a) A look at the integral equation (4.26) reveals why we have only assumed y to be continuous on the half-open interval $(0, h]$ in Theorem 4.2.1 and not on the closed interval $[0, h]$ as we could have done for equations of integer order: If y were continuous throughout $[0, h]$ then the left-hand side of the integral equation is continuous in this interval, and so is the integral on the right-hand side (because of the continuity of f). Therefore, the sum must be continuous on $[0, h]$ too. In view of the definition of n , we easily see that the summands are indeed continuous on $[0, h]$ for $k = 1, 2, \dots, n-1$, but the remaining one ($k = n$) is unbounded as $x \rightarrow 0$ because $n > \alpha$ if $\alpha \notin \mathbb{N}$, unless $b_n = 0$. Thus y cannot be continuous at the origin unless $b_n = 0$.

b) If we argue in the same way for the integral equation (4.27) we can see directly why we assume y to be continuous on the closed interval $[0, h]$ in Theorem 4.2.2: The sum on the right-hand side is continuous, since only non-negative integer order monomials occur, whereas for $k = n$ in (4.26) for the Riemann-Liouville type the term $x^{\alpha-n}$ occur which is singular at 0.

c) At last, by comparing the described initial conditions (4.23) for the Riemann-Liouville fractional differential equations with the ones for the Caputo type (4.25), we note that in the Caputo case the initial conditions are formulated as they are in the classical case of ordinary differential equations (of integer order). While the existence and uniqueness results can be derived for both types of fractional differential equations, this has a rather important impact on applications: Usually the initial condition for the Riemann-Liouville type (4.23) have no obvious meaning in applications and they can not be measured.

Proof: (of Theorem 4.2.3) 1. Assume first that y is a solution of the integral equation. We can rewrite this equation in the shorter form

$$y(x) = \sum_{k=1}^n \frac{b_k x^{\alpha-k}}{\Gamma(\alpha-k+1)} + J_0^\alpha f(\cdot, y(\cdot))(x).$$

Now we apply the differential operator D_0^α to both sides of this relation and immediately obtain, in view of Example 4.1.2 and Theorem 4.1.14, that y also solves the differential equation. With respect to the initial conditions, we look at the case $1 \leq k \leq n-1$ first and find, by an application of $D_0^{\alpha-k}$ to the Volterra equation, that

$$D_0^{n-k}y(x) = \sum_{j=1}^n \frac{b_j D_0^{\alpha-k}(\cdot)^{\alpha-j}(x)}{\Gamma(\alpha-j+1)} + D_0^{\alpha-k} J_0^{\alpha-k} J_0^k f(\cdot, y(\cdot))(x)$$

in view of the semigroup property of fractional integration. By Example 4.1.2 we find that the summands vanish for $j > k$. Moreover, by the same example, the summands for $j < k$ vanish if $x = 0$. Thus, according to Theorem 4.1.14,

$$D_0^{\alpha-k}y(0) = \frac{b_k D_0^{\alpha-k}(\cdot)^{\alpha-k}(0)}{\Gamma(\alpha-k+1)} + J_0^k f(\cdot, y(\cdot))(0).$$

Since $k \geq 1$, the integral vanishes, and once again applying Example 4.1.2 we find that $D_0^{\alpha-k}(\cdot)^{\alpha-k}(x) = \Gamma(\alpha-k+1)$. Thus $D_0^{\alpha-k}y(0) = b_k$ as required by the initial condition. Finally for $k = n$ we apply the operator $J_0^{n-\alpha}$ to both sides of the integral equation and find that, in the limit $z \rightarrow 0$, all the summands of the sum vanish except for the n th. The integral $J_0^{n-\alpha} J_0^\alpha f(\cdot, y(\cdot))(z) = J_0^n f(\cdot, y(\cdot))(z)$ also vanishes as $z \rightarrow 0$. Therefore, we find

$$\lim_{z \rightarrow 0+} J_0^{n-\alpha} y(z) = \lim_{z \rightarrow 0+} J_0^{n-\alpha} \frac{b_n J_0^{n-\alpha}(\cdot)^{\alpha-n}(z)}{\Gamma(\alpha-n+1)} = b_n$$

because of Example 4.1.1. Thus y solves the given initial value problem.

If y is a continuous solution of the initial value problem then we define $z(x) := f(x, y(x))$. By assumption, z is a continuous function and $z(x) = f(x, y(x)) = D^\alpha y(x) = D^n J_0^{n-\alpha} y(x)$. Thus, $D^n J_0^{n-\alpha} y$ is continuous too, i.e. $J_0^{n-\alpha} y \in C^n(0, h]$. We may therefore apply Theorem 4.1.15 to derive

$$y(x) = J_0^\alpha D_0^\alpha y(x) + \sum_{k=1}^n c_k x^{\alpha-k} = J_0^\alpha f(\cdot, y(\cdot))(x) + \sum_{k=1}^n c_k x^{\alpha-k}$$

with certain constants c_1, \dots, c_n . Introducing the initial conditions as indicated above, we can determine these constants c_k as $c_k = b_k / \Gamma(\alpha - k + 1)$.

2. Utilizing the definition of the Caputo differential operator we can rewrite the fractional differential equation (4.24) to

$$f(x, y(x)) = D_*^\alpha y(x) = D^\alpha (y - T_{n-1}[y; 0])(x) = D^n J^{n-\alpha} (y - T_{n-1}[y; 0])(x).$$

As we are dealing with continuous function we can integrate n -times on both sides and get

$$J^n f(x, y(x)) = J^{1-\alpha} (y(x) - T_{n-1}[y; 0])(x) + q(x),$$

where $q(x)$ is a polynomial of degree not exceeding $n-1$. Since $f(x, y(x))$ is continuous $J^n f(x, y(x))$ has an n -fold zero at the origin. By definition of the Taylor polynomial this is

true for the term $J^{1-\alpha}(y - T_{n-1}[y_0; 0])(x)$ as well and due to the equality of the equation also for $q(x)$. Hence $q(x) = 0$ and consequently

$$J^n f(x, y(x)) = J^{n-\alpha}(y - T_{n-1}[y; 0])(x).$$

Applying the Riemann-Liouville operator $D^{n-\alpha}$ on both sides of the equation yields

$$J^\alpha f(x, y(x)) = y(x) - T_{n-1}[y; 0](x),$$

which is the Volterra integral equation (4.27).

The other direction of the equality can be proven by applying the Caputo operator D_*^α on both sides of the Volterra integral equation (4.27) resulting in

$$D_*^\alpha y(x) = D_*^\alpha \left(\sum_{k=0}^{n-1} \frac{x^k}{k!} b_k \right) + D_*^\alpha \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

Because the polynomial lies inside the kernel of the operator D_*^α only the term $D_*^\alpha J^\alpha f(x, y(x))$ remains on the right-hand side, so that the equation reduces to

$$D_*^\alpha y(x) = f(x, y(x)),$$

which is the fractional order differential equation (4.24). In order to check the correctness of the initial conditions we differentiate the equation (4.27) k -times with $k = 0, 1, \dots, n-1$ using the Leibniz rule for the differentiation of an integral for the integral term and get

$$y^{(k)}(x) = \sum_{j=k}^{n-k-1} \frac{x^{j-k}}{(j-k)!} b_k + \frac{c(k)}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-k-1} f(t, y(t)) dt,$$

where the constant $c(k) = \prod_{j=1}^k (\alpha - k)$ contains the terms arising because of the repeated differentiation of the integral. For the cases $k < n-1$ only b_k remains for $x = 0$ because all other terms in the sum except the first one vanish and the integration from 0 to 0 of two continuous functions is zero. In the case $k = n-1$ the integral contains a singularity at the origin and therefore we cannot use this simple explanation. However, exploiting the fact that this integral exists in L^1 we can take the limit and get

$$\lim_{x \rightarrow 0} \int_0^x (x-t)^{\alpha-k-1} f(t, y(t)) ds = 0$$

and therefore again only b_{n-1} remains. Hence the correctness of the initial values is validated. \square

With this result we can now prove analogues to the Theorems 4.2.1 and 4.2.2, where we state the results in terms of the corresponding integral equations:

Lemma 4.2.4 *Under the assumptions of Theorem 4.2.1, the Volterra equation*

$$(4.28) \quad y(x) = \sum_{k=1}^n \frac{b_k x^{\alpha-k}}{\Gamma(\alpha-k+1)} + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt$$

possesses a uniquely determined solution $y \in C(0, h]$.

Proof: We define the set

$$B := \left\{ y \in C(0, h] : \sup_{0 < x \leq h} \left| x^{n-\alpha} y(x) - \sum_{k=1}^n \frac{b_k x^{n-k}}{\Gamma(\alpha - k + 1)} \right| \leq K \right\}$$

and on this set we define the operator A by

$$Ay(x) := \sum_{k=1}^n \frac{b_k x^{\alpha-k}}{\Gamma(\alpha - k + 1)} + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

Then we note that, for $y \in B$, Ay is also a continuous function on $(0, h]$. Moreover,

$$\begin{aligned} \left| x^{n-\alpha} Ay(x) - \sum_{k=1}^n \frac{b_k x^{n-k}}{\Gamma(\alpha - k + 1)} \right| &= \left| \frac{x^{n-\alpha}}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt \right| \\ &\leq \frac{x^{n-\alpha}}{\Gamma(\alpha)} M \int_0^x (x-t)^{\alpha-1} dt \\ &\leq \frac{x^{n-\alpha}}{\Gamma(\alpha)} M \frac{x^\alpha}{\alpha} = \frac{x^n M}{\Gamma(\alpha + 1)} \leq K \end{aligned}$$

for $x \in (0, h]$, where the last inequality follows from the definition of h . This shows that $Ay \in B$ if $y \in B$, i.e. the operator A maps the set B into itself.

Next we introduce a new set

$$\widehat{B} := \left\{ y \in C(0, h] : \sup_{0 < x \leq h} |x^{n-\alpha} y(x)| < \infty \right\},$$

and on this set we define a norm $\|\cdot\|_{\widehat{B}}$ by

$$\|y\|_{\widehat{B}} := \sup_{0 < x \leq h} |x^{n-\alpha} y(x)|.$$

It is easily seen that \widehat{B} , equipped with this norm, is a normed linear space, and that B is a complete subset of this space.

Using the definition of A , we can rewrite the Volterra equation in the more compact form

$$y = Ay.$$

Hence, in order to prove the desired result, it is sufficient to show that the operator A has a unique fixed point. For this purpose, we shall employ Weissinger's fixed point theorem (Theorem 2.1.12). In this context we prove, for $y, \tilde{y} \in B$,

$$(4.29) \quad \|A^j y - A^j \tilde{y}\|_{\widehat{B}} \leq \left(\frac{L h^\alpha \Gamma(\alpha - n + 1)}{\Gamma(2\alpha - n + 1)} \right)^j \|y - \tilde{y}\|_{\widehat{B}}.$$

This can be shown by induction: In the case $j = 0$, the statement is trivially true. For the induction step $j - 1 \mapsto j$, we proceed as follows. We write

$$\|A^j y - A^j \tilde{y}\|_{\widehat{B}}$$

$$\begin{aligned}
&= \sup_{0 < x \leq h} \left| x^{n-\alpha} (A^j y(x) - A^j \tilde{y}(x)) \right| \\
&= \sup_{0 < x \leq h} \left| x^{n-\alpha} (AA^{j-1} y(x) - AA^{j-1} \tilde{y}(x)) \right| \\
&= \sup_{0 < x \leq h} \left| \frac{x^{n-\alpha}}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} [f(t, A^{j-1} y(t)) - f(t, A^{j-1} \tilde{y}(t))] dt \right| \\
&\leq \sup_{0 < x \leq h} \frac{x^{n-\alpha}}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} |f(t, A^{j-1} y(t)) - f(t, A^{j-1} \tilde{y}(t))| dt \\
&\leq \frac{L}{\Gamma(\alpha)} \sup_{0 < x \leq h} x^{n-\alpha} \int_0^x (x-t)^{\alpha-1} |A^{j-1} y(t) - A^{j-1} \tilde{y}(t)| dt
\end{aligned}$$

by definition of the operator A and the Lipschitz condition on f . In the next step we estimate further to find

$$\begin{aligned}
&\|A^j y - A^j \tilde{y}\|_{\widehat{B}} \\
&\leq \frac{L}{\Gamma(\alpha)} \sup_{0 < x \leq h} x^{n-\alpha} \int_0^x (x-t)^{\alpha-1} |A^{j-1} y(t) - A^{j-1} \tilde{y}(t)| dt \\
&\leq \frac{L}{\Gamma(\alpha)} \sup_{0 < x \leq h} x^{n-\alpha} \int_0^x (x-t)^{\alpha-1} t^{\alpha-n} t^{n-\alpha} |A^{j-1} y(t) - A^{j-1} \tilde{y}(t)| dt \\
&\leq \frac{L}{\Gamma(\alpha)} \|A^{j-1} y - A^{j-1} \tilde{y}\|_{\widehat{B}} \sup_{0 < x \leq h} x^{n-\alpha} \int_0^x (x-t)^{\alpha-1} t^{\alpha-n} dt \\
&= \frac{L}{\Gamma(\alpha)} \|A^{j-1} y - A^{j-1} \tilde{y}\|_{\widehat{B}} \sup_{0 < x \leq h} \frac{\Gamma(\alpha)\Gamma(\alpha-n+1)}{\Gamma(2\alpha-n+1)} x^\alpha \\
&= \frac{Lh^\alpha \Gamma(\alpha-n+1)}{\Gamma(2\alpha-n+1)} \|A^{j-1} y - A^{j-1} \tilde{y}\|_{\widehat{B}}.
\end{aligned}$$

Now we use the induction hypothesis, proving (4.29). Therefore, we may apply Theorem 2.1.12 with $\alpha_j = \gamma^j$ where $\gamma = (Lh^\alpha \Gamma(\alpha-n+1)/\Gamma(2\alpha-n+1))^j$. It remains to prove that the series $\sum_{j=0}^\infty \alpha_j$ is convergent. This, however, is trivial in view of the fact that $h \leq \tilde{h}$ and the definition of \tilde{h} that implies $\gamma < 1$. Thus an application of the fixed point theorem yields the existence and the uniqueness of the solution of our integral equation. \square

Lemma 4.2.5 *Under the assumptions of Theorem 4.2.2, the Volterra equation*

$$(4.30) \quad y(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} D^k y(0) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

possesses a uniquely determined solution $y \in C[0, h]$.

Proof: We divide the proof in two parts. First we consider the case $\alpha > 1$ and secondly the case $\alpha \in (0, 1)$. The reasoning behind this lies in the fact that the Volterra integral equation (4.30) possesses a singular kernel $(x-t)^{\alpha-1}$ in the case $\alpha \in (0, 1)$, while the kernel is continuous in the other case.

Case $\alpha > 1$: The equation (4.30) possesses a continuous kernel and a continuous given function outside the integral. Thus the existence of the solution follows using standard methods from the theory of Volterra equations [106, §II.1]. Similarly by using the Lipschitz condition the uniqueness can be proven directly with standard methods from the theory of Volterra equations [106, §II.1].

Case $\alpha \in (0, 1)$: In this situation, the Volterra equation (4.30) reduces to

$$(4.31) \quad y(x) = b_0 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

For the proof of the existence of a solution we introduce the set

$$U := \{y \in C[0, h] : \|y - b_0\|_\infty \leq K\}.$$

Obviously, this is a closed and convex subset of the Banach space of all continuous functions on $[0, h]$, equipped with the Chebyshev norm. Since the constant function $y \equiv b_0$ is in U , we also see that U is not empty. On U we define the operator A by

$$(4.32) \quad (Ay)(x) := b_0 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

Using this operator, the equation under consideration can be rewritten as

$$y = Ay,$$

and in order to prove our desired existence result, we have to show that A has a fixed point. Let us therefore investigate the properties of the operator A .

First we note that, for $0 \leq x_1 \leq x_2 \leq h$,

$$\begin{aligned} |(Ay)(x_1) - (Ay)(x_2)| &= \frac{1}{\Gamma(\alpha)} \left| \int_0^{x_1} (x_1-t)^{\alpha-1} f(t, y(t)) dt \right. \\ &\quad \left. - \int_0^{x_2} (x_2-t)^{\alpha-1} f(t, y(t)) dt \right| \\ &= \frac{1}{\Gamma(\alpha)} \left| \int_0^{x_1} \left((x_1-t)^{\alpha-1} - (x_2-t)^{\alpha-1} \right) f(t, y(t)) dt \right. \\ &\quad \left. + \int_{x_1}^{x_2} (x_2-t)^{\alpha-1} f(t, y(t)) dt \right| \\ &\leq \frac{\|f\|_\infty}{\Gamma(\alpha)} \left| \int_0^{x_1} \left((x_1-t)^{\alpha-1} - (x_2-t)^{\alpha-1} \right) dt \right. \\ &\quad \left. + \int_{x_1}^{x_2} (x_2-t)^{\alpha-1} dt \right| \\ (4.33) \quad &= \frac{\|f\|_\infty}{\Gamma(\alpha+1)} (2(x_2-x_1)^\alpha + x_1^\alpha - x_2^\alpha), \end{aligned}$$

proving that Ay is a continuous function. Moreover, for $y \in U$ and $x \in [0, h]$, we find

$$\begin{aligned} |(Ay)(x) - y_0^{(0)}| &= \frac{1}{\Gamma(\alpha)} \left| \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt \right| \leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty x^\alpha \\ &\leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty h^\alpha \leq \frac{1}{\Gamma(\alpha+1)} \|f\|_\infty \frac{K\Gamma(\alpha+1)}{\|f\|_\infty} = K. \end{aligned}$$

Thus, we have shown that $Ay \in U$ if $y \in U$, i.e. A maps the set U to itself.

Since we want to apply Schauder's Fixed Point Theorem (Theorem 2.1.14), all that remains now is to show that $A(U) := \{Au : u \in U\}$ is a relatively compact set. This can be done by means of the Arzelà-Ascoli Theorem (Theorem 2.1.15). For $z \in A(U)$ we find that, for all $x \in [0, h]$,

$$\begin{aligned} |z(x)| &= |(Ay)(x)| \leq |b_0| + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} |f(t, y(t))| dt \\ &\leq |b_0| + \frac{1}{\Gamma(\alpha+1)} \|f\|_{\infty} h^{\alpha}, \end{aligned}$$

which is the required boundedness property. Moreover, for $0 \leq x_1 \leq x_2 \leq h$, we have found above, cf. equation (4.33), that

$$\begin{aligned} |(Ay)(x_1) - (Ay)(x_2)| &\leq \frac{\|f\|_{\infty}}{\Gamma(\alpha+1)} (x_1^{\alpha} - x_2^{\alpha} + 2(x_2 - x_1)^{\alpha}) \\ &\leq 2 \frac{\|f\|_{\infty}}{\Gamma(\alpha+1)} (x_2 - x_1)^{\alpha}. \end{aligned}$$

Thus, if $|x_2 - x_1| < \delta$, then

$$|(Ay)(x_1) - (Ay)(x_2)| \leq 2 \frac{\|f\|_{\infty}}{\Gamma(\alpha+1)} \delta^{\alpha}.$$

Noting that the expression on the right-hand side is independent of y , we see that the set $A(U)$ is equicontinuous. Then, the Arzelà-Ascoli Theorem yields that $A(U)$ is relatively compact. Thus, Schauder's Fixed Point Theorem asserts that A has got a fixed point. By construction, a fixed point of A is a solution of our initial value problem.

For the uniqueness of the solution we use the operator A again and recall that it maps the nonempty, convex and closed set $U = \{y \in C[0, h] : \|y - b_0\|_{\infty} \leq K\}$ to itself. We now have to prove that A has got a unique fixed point. In order to do this, we shall first prove that, for every $j \in \mathbb{N}_0$ and every $x \in [0, h]$, we have

$$(4.34) \quad \|A^j y - A^j \tilde{y}\|_{L_{\infty}[0, x]} \leq \frac{(Lx^{\alpha})^j}{\Gamma(1 + \alpha j)} \|y - \tilde{y}\|_{L_{\infty}[0, x]}.$$

This can be seen by induction. In the case $j = 0$, the statement is trivially true. For the induction step $j - 1 \mapsto j$, we write

$$\begin{aligned} &\|A^j y - A^j \tilde{y}\|_{L_{\infty}[0, x]} \\ &= \|A(A^{j-1}y) - A(A^{j-1}\tilde{y})\|_{L_{\infty}[0, x]} \\ &= \frac{1}{\Gamma(\alpha)} \sup_{0 \leq w \leq x} \left| \int_0^w (w-t)^{\alpha-1} [f(t, A^{j-1}y(t)) - f(t, A^{j-1}\tilde{y}(t))] dt \right|. \end{aligned}$$

In the next steps, we use the Lipschitz assumption on f and the induction hypothesis and find

$$\begin{aligned}
& \left\| A^j y - A^j \tilde{y} \right\|_{L_\infty[0,x]} \\
& \leq \frac{L}{\Gamma(\alpha)} \sup_{0 \leq w \leq x} \int_0^w (w-t)^{\alpha-1} \left| A^{j-1} y(t) - A^{j-1} \tilde{y}(t) \right| dt \\
& \leq \frac{L}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} \sup_{0 \leq w \leq t} \left| A^{j-1} y(w) - A^{j-1} \tilde{y}(w) \right| dt \\
& \leq \frac{L^j}{\Gamma(\alpha)\Gamma(1+\alpha(j-1))} \int_0^x (x-t)^{\alpha-1} t^{\alpha(j-1)} \sup_{0 \leq w \leq t} |y(w) - \tilde{y}(w)| dt \\
& \leq \frac{L^j}{\Gamma(\alpha)\Gamma(1+\alpha(j-1))} \sup_{0 \leq w \leq x} |y(w) - \tilde{y}(w)| \int_0^x (x-t)^{\alpha-1} t^{\alpha(j-1)} dt \\
& = \frac{L^j}{\Gamma(\alpha)\Gamma(1+\alpha(j-1))} \|y - \tilde{y}\|_{L_\infty[0,x]} \frac{\Gamma(\alpha)\Gamma(1+\alpha(j-1))}{\Gamma(1+\alpha j)} x^{\alpha j}
\end{aligned}$$

which is our desired result (4.34). As a consequence, we find, taking Chebyshev norms on our fundamental interval $[0, h]$,

$$\left\| A^j y - A^j \tilde{y} \right\|_\infty \leq \frac{(Lh^\alpha)^j}{\Gamma(1+\alpha j)} \|y - \tilde{y}\|_\infty.$$

We have now shown that the operator A fulfills the assumptions of Theorem 2.1.12 with $\alpha_j = (Lh^\alpha)^j / \Gamma(1+\alpha j)$. In order to apply that theorem, we only need to verify that the series $\sum_{j=0}^\infty \alpha_j$ converges. This, however, follows immediately from Theorem 3.4.1 property 3. Therefore, we may apply Weissinger's Fixed Point Theorem and deduce the uniqueness of the solution of our differential equation. \square

It is apparent that the expression $\sum_{j=0}^\infty \alpha_j$ from the proof of Theorem 4.2.5 is nothing but $E_\alpha(Lh^\alpha)$. The Mittag-Leffler functions do not only arise in this context; they actually play a very important role in the entire field of fractional calculus. For the moment we only state the most prominent result in this context explicitly.

Theorem 4.2.6 *Let $\alpha > 0$, $n = \lceil \alpha \rceil$ and $\lambda \in \mathbb{R}$. The solution of the initial value problem*

$$D_*^\alpha y(x) = \lambda y(x), \quad y(0) = 1, \quad y^{(k)}(0) = 0 \quad (k = 1, 2, \dots, n-1)$$

is given by

$$y(x) = E_\alpha(\lambda x^\alpha), \quad x \geq 0.$$

In other words, the eigenfunctions of the Caputo differential operators may be expressed in terms of Mittag-Leffler functions.

Proof: It is evident from our existence and uniqueness theorems above that the initial value problem has a unique solution. Therefore, we only have to verify that the function y stated above is a solution. For the initial condition, we see indeed that $y(0) = E_\alpha(0) = 1$ since

$$E_\alpha(\lambda x^\alpha) = 1 + \frac{\lambda x^\alpha}{\Gamma(1+\alpha)} + \frac{\lambda^2 x^{2\alpha}}{\Gamma(1+2\alpha)} + \dots;$$

moreover, in the case $n \geq 2$ (i.e. $\alpha > 1$) we have $y^{(k)}(0) = 0$ for $k = 1, 2, \dots, n-1$ since

$$y(x) = 1 + \frac{\lambda x^\alpha}{\Gamma(1+\alpha)} + \frac{\lambda^2 x^{2\alpha}}{\Gamma(1+2\alpha)} + \dots$$

which implies that

$$y^{(k)}(x) = \frac{\lambda x^{\alpha-k}}{\Gamma(1+\alpha-k)} + \frac{\lambda^2 x^{2\alpha-k}}{\Gamma(1+2\alpha-k)} + \dots$$

for $k = 1, 2, \dots, n-1 < \alpha$.

Concerning the differential equation, we first look at the case $\lambda = 0$ and note that in this case $y(x) = E_\alpha(0) = 1$. Hence, $D_*^\alpha y(x) = 0 = \lambda y(x)$ as required. If, on the other hand, $\lambda \neq 0$, then (using the notation $p_k(x) := x^k$)

$$\begin{aligned} D_*^\alpha y(x) &= D_*^\alpha \left[\sum_{j=0}^{\infty} \frac{(\lambda p_\alpha)^j}{\Gamma(1+j\alpha)} \right] (x) = J_0^{n-\alpha} D^n \left[\sum_{j=0}^{\infty} \frac{\lambda^j p_{\alpha j}}{\Gamma(1+j\alpha)} \right] (x) \\ &= J_0^{n-\alpha} \left[\sum_{j=0}^{\infty} \frac{\lambda^j D^n p_{\alpha j}}{\Gamma(1+j\alpha)} \right] (x) = J_0^{n-\alpha} \left[\sum_{j=1}^{\infty} \frac{\lambda^j D^n p_{\alpha j}}{\Gamma(1+j\alpha)} \right] (x) \\ &= J_0^{n-\alpha} \left[\sum_{j=1}^{\infty} \frac{\lambda^j p_{\alpha j-n}}{\Gamma(1+j\alpha-n)} \right] (x) = \sum_{j=1}^{\infty} \frac{\lambda^j J_0^{n-\alpha} p_{\alpha j-n}(x)}{\Gamma(1+j\alpha-n)} \\ &= \sum_{j=1}^{\infty} \frac{\lambda^j p_{\alpha j-n}(x)}{\Gamma(1+j\alpha-n)} = \sum_{j=1}^{\infty} \frac{\lambda^j x^{\alpha j-n}}{\Gamma(1+j\alpha-n)} \\ &= \sum_{j=0}^{\infty} \frac{\lambda^{j+1} x^{\alpha j}}{\Gamma(1+j\alpha)} = \lambda \sum_{j=0}^{\infty} \frac{(\lambda x^\alpha)^j}{\Gamma(1+j\alpha)} = \lambda y(x). \end{aligned}$$

Here we have used the fact that, in view of the convergence properties of the series defining the Mittag-Leffler function, we may interchange first summation and differentiation and later summation and integration. \square

4.2.1 Properties of the solution¹

We have seen in Theorem 4.2.3 that fractional order differential equations can be treated as a special form of Volterra integral equations. In this section we want to prove some analytic results on the solution of those integral equations. We will state these results for the general case of Abel-Volterra integral equations and thus we start with a formal definition.

Definition 4.2.2 *An equation of the form*

$$(4.35) \quad y(x) = f(x) + \int_0^x (x-t)^\alpha K(x, t, y(t)) dt, \quad x \in [0, X]$$

with $\alpha > -1$ and some $X > 0$ is called Volterra integral equation with weak singularity in the kernel.

Remark 4.2.2 *The parameter α in the Volterra integral equation (4.35) is not exactly the parameter α in the Volterra integral equations (4.26) and (4.27) arising from the fractional differential equations of Riemann-Liouville or Caputo type respectively. Of course, a simple transformation $\alpha \rightarrow \alpha - 1$ in (4.35) and splitting the parameter $1/\Gamma(\alpha)$ from the kernel K in (4.35) points out the connection of fractional order differential equations and the Volterra integral equation in (4.35). In this chapter we use representation (4.35) since the results we are going to present are corrected versions of results in [94], where the Volterra integral equation is defined as in Definition 4.2.2.*

The Volterra integral equations (4.26) and (4.27) obtained from fractional order differential equations of either Riemann-Liouville or Caputo type are thus special cases of the general Volterra integral equation, where the forcing function $f(x)$ and the kernel $K(x, t, y(t))$ have a special structure.

As we will see in Chapter 5.1.3 the knowledge of the smoothness properties of the solution of the integral equation (4.35) is indispensable for the construction of a certain type of numerical methods. Some important statements on this topic are given in the fundamental paper of Lubich [94]. Unfortunately it turns out that not all of these statements are true as shown in a paper by Diethelm et al [40]. Thus we point out these errors in the following theorems and give corrected versions of the results.

Remark 4.2.3 *In the following results the solution of equation (4.35) is assumed to be continuous in the complex neighbourhood of the interval $(0, X)$ when needed. For the numerical algorithms developed later in this thesis the assumptions of a continuous solution on the interval $[0, X]$ would be sufficient since only the expansion of the solution at the origin is needed in those cases. However, to obtain the general results regarding the properties of the solution on the whole given interval one has to take the possible occurrence of singularities in the interval in question into consideration.*

A fundamental result of Lubich, given in [94, Thm. 2], yields structural information on the behaviour of the solution y of the Volterra equation (4.35) near the origin. Specifically,

¹Some results in this chapter were found to be incorrect in studies on this subject after this thesis was finished. Newer results will be published in a revised version of [40]

it is claimed that the solution is of the form $y(x) = Y(x, x^{\alpha+1})$ with a bivariate function Y that is analytic at the origin if K is analytic at the origin and $f(x) = F(x, x^{\alpha+1})$ with some function F that is also analytic at the origin. It is evident that the basic error is the assumption that K should be analytic at the origin. A correct formulation reads as follows.

Theorem 4.2.7 *Consider the Volterra equation (4.35) with non-integer α , assume that K is analytic in a neighbourhood of the point $(0, 0, f(0))$ and $f(x) = F(x, x^{\alpha+1})$ where $F(z_1, z_2)$ is analytic in a neighbourhood of $(0, 0)$. Then, there exists an analytic function $Y(z_1, z_2)$ with $y(x) = Y(x, x^{\alpha+1})$.*

Proof: The proof is taken from [94]. We repeat the main ideas for convenience. The only major change is to leave out the assumption $f(0) = 0$ made in [94]. As it was shown in [94], it is no loss of generality to assume that K is of the form

$$K(x, t, y) = K(x, y) = \sum_{k \in \mathbb{N}_0} K_k(x)(y - f(0))^k.$$

We substitute the ansatz

$$A(z_1, z_2) = f(0) + \sum_{(n_1, n_2) \in N} a_{(n_1, n_2)} z_1^{n_1} z_2^{n_2}$$

into equation (4.35), where $N = \mathbb{N}_0^2 \setminus \{(0, 0)\}$ and $A(z_1, z_2)$ is an analytic function.

Because of the uniform convergence we can interchange the sums and the integral, so we obtain

$$\begin{aligned} & \int_0^x (x-t)^\alpha K(x, A(t, t^{\alpha+1})) dt \\ &= \sum_k K_k(x) \sum_{(n_1, n_2) \in N} P_{k, (n_1, n_2)}(A) \int_0^x (x-t)^\alpha t^{n_1} (t^{\alpha+1})^{n_2} dt. \end{aligned}$$

The $P_{k, (n_1, n_2)}(A)$ are polynomials in the coefficients $a_{(n_1, n_2)}$ of the ansatz and the integrals can be evaluated in terms of the well known Beta function given in Definition 3.3.1.

These calculations show that a formal solution is given using the power series

$$(4.36) \quad Y(z_1, z_2) = F(z_1, z_2) + z_2 \sum_N \hat{B}(n_1, n_2) \sum_k K_k(x) P_{k, (n_1, n_2)}(Y) z_1^{n_1} z_2^{n_2},$$

with the relations $z_1 = x$, $z_2 = x^{\alpha+1}$ and $\hat{B}(n_1, n_2) = B(1 + \alpha, 1 + n_1 + n_2(1 + \alpha))$, where B is the Beta function. With the help of the analytic version of the implicit function theorem and convergent majorants of F and K this formal series can be shown to converge. This means that $y(x) = Y(x, x^{\alpha+1})$ with $Y(z_1, z_2)$ given by equation (4.36) is the solution to our problem. \square

A direct consequence of this theorem (see also [94, Cor. 3]) is given by

Corollary 4.2.8 *If the function F with $f(x) = F(x, x^{1+\alpha})$ and the kernel K are only assumed to be sufficiently differentiable, then the solution $y(x)$ of (4.35) has an asymptotic expansion in mixed powers of x and $x^{1+\alpha}$ as $x \rightarrow 0$.*

The next example not only shows why the version of Theorem 4.2.7 given by Lubich goes wrong, but reveals possible properties of the counterexamples that are in interesting contrast to the problems that satisfy the assumptions made in [94].

Example 4.2.1 *Consider the integral equation*

$$(4.37) \quad y(x) = 1 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} \frac{1}{y(t)-1} dt$$

with non-integer α and $0 < \alpha < 2$. This equation corresponds to the initial value problems

$$(4.38) \quad D_*^\alpha y(x) = \frac{1}{y(x)-1}, \quad y(0) = 1,$$

for $0 < \alpha < 1$ and

$$(4.39) \quad D_*^\alpha y(x) = \frac{1}{y(x)-1}, \quad y(0) = 1, y'(0) = 0,$$

for $1 < \alpha < 2$. Equation (4.37) is solved by the functions

$$(4.40) \quad y(x) = 1 \pm \frac{\sqrt{\Gamma(1-\alpha/2)}}{\sqrt{\Gamma(1+\alpha/2)}} x^{\alpha/2},$$

which is readily verified by substitution. The equation

$$y(x) = 1 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} \frac{1}{1-y(t)} dt$$

is solved by

$$y(x) = 1 \pm i \frac{\sqrt{\Gamma(1-\alpha/2)}}{\sqrt{\Gamma(1+\alpha/2)}} x^{\alpha/2}.$$

Several points are important to note from this example

Remark 4.2.4 *a) Because the solutions to the problem “start” in the singularity of the right-hand side of the differential equation, Theorem 4.2.7 is not applicable. The different structure of the solutions compared to problems which satisfy the requirements of Theorem 4.2.7 suggests the distinction between “regular” and “singular” initial value problems.*

b) While Theorem 4.2.7 and Corollary 4.2.8 reveal the structure of the solutions of regular problems, Example 4.2.1 shows that they fail for singular ones. Classical numerical methods of high order, such as those developed by Lubich in [95], strongly depend on these structural properties of the solutions and therefore do not perform well in the case of singular kernels K , see Chapter 6.3.

c) The integral equation (4.37) and the initial value problem (4.39) are not equivalent because the integral equation has solutions that are not differentiable at the origin. This is caused by the singularity of the given function on the right-hand side of the differential equation.

It is commonly believed that for non-integer values α the Kernel function K cannot be smooth if the solution is smooth, and vice versa. This is supported by the remark of Lubich [94, p. 89], referring to the Volterra equation with an analytic kernel K , that “it is easily seen that $f(x)$ and $y(x)$ cannot be smooth at 0 simultaneously”. In general a very detailed analysis of the smoothness properties of the solutions is available [94, 107] (which need to be interpreted in the light of Theorem 4.2.7 above), and these results indicate that y should be of the form $y(x) = Y(x, x^{\alpha+1})$ with Y being an analytic function of two variables. Therefore, y consists of smooth and non-smooth parts, and we shall now give a precise account of when all the non-smooth parts vanish, leaving an analytic solution:

Theorem 4.2.9 *Consider the Volterra equation (4.35) with non-integer α , and assume that K is analytic on a suitable set G and that f is analytic on $[0, X]$. Then, y is analytic if and only if $K(x, t, f(t)) = 0$ for all $x, t \in [0, X]$.*

Proof: We first note that the analyticity of K implies the existence of a unique solution.

The direction “ \Leftarrow ” is a simple consequence of the fact that a solution (and hence, by uniqueness, *the* solution) of the initial value problem is $y = f$ because then the left-hand side of equation (4.35) is $f(x)$, whereas the right-hand side has the value

$$f(x) + \int_0^x (x-t)^\alpha K(x, t, f(t)) dt = f(x).$$

Hence the solution is analytic.

For the other direction, we assume y to be analytic. Then, since K is analytic, the function $z : [0, X]^2 \rightarrow \mathbb{R}$ with $z(x, t) := K(x, t, y(t))$ is analytic too. Let us now assume that this function z is not identically zero. Recalling that the integrand is the product of this analytic function z and the non-analytic function $(x-t)^\alpha$, we note that the full integrand is not analytic, and hence the integral (as a function of x) is not analytic either. But in view of the Volterra equation, we have that the integral is identical to $y - f$, which is an analytic function. Hence we obtain a contradiction.

As a consequence, we derive that $0 = z(x, t) = K(x, t, y(t))$ for all x and t . We can insert this relation into the Volterra equation and find that

$$y(x) = f(x) + \int_0^x (x-t)^\alpha K(x, t, y(t)) dt = f(x)$$

for all x , and therefore we conclude $0 = z(x, t) = K(x, t, y(t)) = K(x, t, f(t))$ for all x and t . \square

Of course the condition $K(x, t, f(t)) = 0$ is easy to check in practice because it only involves given functions. We point out two immediate corollaries of Theorem 4.2.9.

Corollary 4.2.10 *Assume the hypotheses of Theorem 4.2.9. If y is analytic then $y = f$.*

Corollary 4.2.11 *Consider the initial value problem (4.24)(4.25) with an analytic function f , and define $T(x) := \sum_{j=0}^{n-1} y_0^{(j)} x^j / j!$. This problem has an analytic solution y if and only if $f(x, T(x)) = 0$ for all x . Moreover, if y is analytic then $y = T$, i.e. y is the polynomial from the kernel of the Caputo differential operator that fits the initial conditions.*

A simple example clarifies these results:

Example 4.2.2 Consider the integral equation

$$y(x) = x + 1 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} (y-t-1) dt$$

with non-integer α and $1 < \alpha < 2$. This equation corresponds to the initial value problem

$$D_*^\alpha y(x) = y(x) - x - 1, \quad y(0) = 1, y'(0) = 1,$$

and is solved by

$$y(x) = x + 1,$$

which is an analytic function itself.

In many applications, the functions under consideration have a certain number of continuous derivatives, but they are not necessarily analytic. We will state now some results based on these weaker assumptions. For convenience we note that equation (4.35) reads

$$(4.41) \quad y(x) = f(x) + \Gamma(\alpha + 1) J_0^{\alpha+1} [K(x, \cdot, y(\cdot))](x),$$

where $J^{\alpha+1}$ is the Riemann-Liouville integral operator. By a renormalization of the kernel function K we can rewrite this in the form

$$(4.42) \quad y(x) = f(x) + J_0^\beta [K(x, \cdot, y(\cdot))](x),$$

without changing the differentiability properties of the functions involved, so we will analyze the latter.

If β is an integer, the next result is easily proved:

Theorem 4.2.12 Let $k \in \mathbb{N}$, $\beta > 0$, $\beta \in \mathbb{N}$ and an equation of the form (4.42) be given. If $f \in C^{\beta+k}[0, X]$ and $K \in C^k([0, X] \times [0, X] \times \mathbb{R})$, then $y \in C^{\beta+k}[0, X]$.

This result is well-known for ordinary differential equations, but cannot be maintained for non-integer β , cf. [94, 107]. The main problem is the different structure of the solutions at the origin. This behaviour will be analyzed in greater detail now.

In the trivial case where the function K does not depend on the solution, we get the following result:

Theorem 4.2.13 Let $k \in \mathbb{N}$, $\beta > 0$, $\beta \notin \mathbb{N}$ and an equation of the form (4.42) be given, where K does not depend on the solution y . If $f \in C^{[\beta]+k}[0, X]$, $K \in C^k([0, X] \times [0, X])$ and $\left[\frac{\partial^j}{\partial t^j} K(x, t) \right]_{t=0} \in C^{[\beta]+k}[0, X]$, then $y \in C^{[\beta]+o^*}[0, X] \cap C^{[\beta]+k}(0, X)$. Here $o^* = \min\{o, k\}$ where $o \in \mathbb{N}_0$ is defined by

$$\left[\frac{\partial^\mu}{\partial t^\mu} K(x, t) \right]_{x=t=0} \begin{cases} = 0 & \text{for } \mu = 0, 1, \dots, o-1, \\ \neq 0 & \text{for } \mu = o. \end{cases}$$

Proof: Partially integrating the given integral equation k times with respect to t yields

$$\begin{aligned} y(x) = & f(x) + \sum_{j=0}^{k-1} \frac{x^{\beta+j}}{\beta(\beta+1)\cdots(\beta+j)} \left[\frac{\partial^j}{\partial t^j} K(x, t) \right]_{t=0} \\ & + \frac{1}{\Gamma(\beta+k)} \int_0^x (x-t)^{\beta-1+k} \frac{\partial^k}{\partial t^k} K(x, t) dt. \end{aligned}$$

Our assumptions imply $f \in C^{[\beta]+k}[0, X]$ and that the sum is in $C^{[\beta]+o^*}[0, X] \cap C^{[\beta]+k}(0, X)$. Using the semigroup property of the Riemann-Liouville operator we see that the integral operator in the last term is equal to $J^{[\beta]+k} J^{\beta-[\beta]}$. As its argument is continuous by assumption, the complete last term is $J_0^{[\beta]+k}$ applied to a continuous function and so this function is an element of $C^{[\beta]+k}[0, X]$, which completes the proof. \square

If $\beta > 1$ this Theorem can be extended by elementary means.

Theorem 4.2.14 *Let $k \in \mathbb{N}$, $\beta > 1$, $\beta \notin \mathbb{N}$ and an equation of the form (4.42) be given. If $f \in C^{[\beta]+k}[0, X]$, $K \in C^k([0, X] \times [0, X] \times \mathbb{R})$, $\left[\frac{d^j}{dt^j} K(x, t, y(t)) \right]_{t=0} \in C^{[\beta]+k}[0, X]$ and K is of the form $K(x, t, y) = \sum_{i=0}^{k-1} K_i(x)(y - f(0))^i + K_k(x)O((y - f(0))^k)$ with $K_j \in C^{[\beta]+k}[0, X]$ for $0 \leq j \leq k$, then*

$$y \in C^{[\beta]+o^*}[0, X] \cap \begin{cases} C^{[\beta]+k}(0, X) & \text{if } k \leq [\beta], \\ C^{[\beta]+k-1}(0, X) & \text{if } k > [\beta]. \end{cases}$$

As remarked in the proof of Theorem 4.2.7 above, the special choice of K is no loss of generality.

At first sight the hypotheses of this theorem seem rather complicated. However, in some important special cases we can simplify them drastically. Indeed, if the kernel K is independent of x (this case arises, e.g., if the Volterra equation is obtained from a fractional differential equation as in equation (4.27)), then the functions K_1, \dots, K_k and $\left[\frac{d^j}{dt^j} K(x, t, y(t)) \right]_{t=0}$ ($0 \leq j \leq k$) are actually constant and hence they automatically satisfy the required differentiability assumptions. Thus we obtain an immediate consequence of Theorem 4.2.14:

Corollary 4.2.15 *Let $k \in \mathbb{N}$, $\beta > 1$, $\beta \notin \mathbb{N}$ and an equation of the form*

$$y(x) = f(x) + J_0^\beta [K(\cdot, y(\cdot))](x)$$

be given. If $f \in C^{[\beta]+k}[0, X]$ and $K \in C^k([0, X] \times \mathbb{R})$ then

$$y \in C^{[\beta]+o^*}[0, X] \cap \begin{cases} C^{[\beta]+k}(0, X) & \text{if } k \leq [\beta], \\ C^{[\beta]+k-1}(0, X) & \text{if } k > [\beta]. \end{cases}$$

In this corollary it is not necessary to demand a special form of K as in Theorem 4.2.14 explicitly because of the properties mentioned above and the observation indicated in the proof of Theorem 4.2.7.

Proof: (of Theorem 4.2.14) First we note that any continuous solution of an equation of type (4.42) is of class $C^{[\beta]}[0, X]$. This is clear because

$$J_0^{\beta-[\beta]}[K(x, \cdot, y(\cdot))](x)$$

is a continuous function and

$$y(x) = f(x) + J_0^{[\beta]} J_0^{\beta-[\beta]}[K(x, \cdot, y(\cdot))](x).$$

Iteration of this reasoning gives the corresponding Theorem if β is an integer.

As $y \in C^{[\beta]}[0, X]$, we can use partial integration with respect to t again. For $k > [\beta]$ we obtain:

$$\begin{aligned} y(x) &= f(x) + \sum_{j=0}^{[\beta]-1} \frac{x^{\beta+j}}{\beta(\beta+1) \cdots (\beta+j)} \left[\frac{d^j}{dt^j} K(x, t, y(t)) \right]_{t=0} \\ &\quad + \frac{1}{\Gamma(\beta+[\beta])} \int_0^x (x-t)^{[\beta]+\beta-1} \frac{d^{[\beta]}}{dt^{[\beta]}} K(x, t, y(t)) dt. \end{aligned}$$

This equation can be discussed as in Theorem 4.2.13 to obtain $y \in C^{[\beta]+o^*}[0, X] \cap C^{2[\beta]+o^*}(0, X)$ for $k > [\beta]$.

Now we utilize the structure of the solutions near the origin given in [94, Corollary 3], corrected in view of Theorem 4.2.7, to complete the proof for $k > [\beta]$.

By our assumption K is of the form

$$K(x, t, y) = \sum_{i=0}^{k-1} K_i(x)(y - f(0))^i + K_k(x)O((y - f(0))^k),$$

where $O(g(x))$ denotes the Landau symbol and the K_i are of class $C^{[\beta]+k}[0, X]$. Because $\beta > 1$, Corollary 3 in [94] implies that the solution has the form of a finite sum in addition to a term of high order:

$$y(x) = \sum_{m,n} y_{m,n} x^{m+n\beta} + O(x^k).$$

A necessary condition for y to be a solution is $y_{00} = f(0)$. Inserting this in the given equation, using the form of K and changing the order of integral and sum therefore gives:

$$\begin{aligned} y(x) &= f(x) + \sum_{i=0}^{k-1} K_i(x) \left(\sum_{m^*, n^*} y_{m^*, n^*} x^{m^*+n^*\beta} + \int_0^x (x-t)^{\beta-1} O(t^k) dt \right) \\ &\quad + K_k(x) \left(\sum_{k \leq r \leq k\beta} y_r x^r + \int_0^x (x-t)^{\beta-1} O(t^{k+1}) dt \right). \end{aligned}$$

According to the second part of the proof, some of the terms outside of the integrals may vanish. Here we only need to discuss the differentiability on $(0, X]$, so the integrals on the right-hand side are the only crucial terms.

Because of the second part of the proof and the structure of the kernel, we know that both integrands are of class $C^{2[\beta]+o}[0, X]$ and have a zero of order $k-1$ at the origin. This means we can use iterated partial integration with respect to t as in Theorem 4.2.13 to see that the integrals are of class $C^{3[\beta]+o}[0, X]$ (if $k \geq 2[\beta] + o + 1$). But this implies $y \in C^{3[\beta]+o}(0, X]$, which means that the integrands are of class $C^{3[\beta]+o}[0, X]$, so the integrals are smoother indeed.

The process can be iterated to see that the integrals are of class $C^{[\beta]+k-1}[0, X]$ and $C^{[\beta]+k}[0, X]$ respectively.

The case $k < [\beta]$ can be handled using only the first two parts of the proof. \square

With this corollary we will end this section on the properties of the solution of Volterra integral equations. In the next section we will consider fractional versions of linear multistep methods described in Chapter 2.2 for the integer order case. These results will in parts be based on the just stated results, in particular on Theorem 4.2.7.

4.3 Fractional linear multistep methods

We had seen in Lemma 2.2.6 that we can use a convolution quadrature to describe a linear multistep method for integer order integrals. We remind ourselves that in case of a linear multistep method we are interested in a solution y on a closed interval $[0, X]$ for some $X > 0$ and that we seek a solution on a prescribed set of nodes in this interval. These nodes are arranged equispaced inside the interval $[0, X]$ and on its border with a given stepsize h and are additionally assumed to be numbered increasingly x_0, x_1, \dots, x_N , where $N = X/h$, $x_0 = 0$ and $x_N = X$. We expand this idea to include fractional order integrals based on the definitions and theorems in article [96]:

Definition 4.3.1 Let $f : [0, X] \rightarrow \mathbb{C}$. An approximation to the integral equation

$$(4.43) \quad y(x) = (J^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-s)^{\alpha-1} f(s) ds, \quad x \in [0, X]$$

given by

$$(4.44) \quad ({}_h J^\alpha f)(x_n) = h^\alpha \sum_{j=0}^n \omega_{n-j} f(jh) + h^\alpha \sum_{j=0}^s w_{nj} f(jh), \quad n = 0, 1, \dots, N$$

with some fixed $s \in \mathbb{N}$ is called fractional convolution quadrature ω . The weights ω_j are called convolution weights and the term

$${}_h \Omega^\alpha f(x) := h^\alpha \sum_{j=0}^n \omega_{n-j} f(jh), \quad x = nh$$

is called convolution part with corresponding convolution quadrature error given by

$${}_h E^\alpha = {}_h \Omega^\alpha - J^\alpha.$$

The term

$${}_h S^\alpha f(x) := h^\alpha \sum_{j=0}^s w_{nj} f(jh)$$

is called starting part and the weights w_{nj} starting weights.

For the next results on fractional convolution quadrature the concepts of Definition 2.2.5 will be expanded to include fractional convolution quadratures. Again $\omega(\zeta)$ denotes the generating function of the convolution weights ω_j as in Lemma 2.2.6:

Definition 4.3.2 1. A fractional convolution quadrature is stable (for J^α) if

$$\omega_n = O(n^{\alpha-1}).$$

2. A fractional convolution quadrature is consistent of order p (for J^α) if

$$h^\alpha \omega(e^{-h}) = 1 + O(h^p).$$

3. A fractional convolution quadrature is convergent of order p (to J^α) if

$$(4.45) \quad ({}_h E^\alpha x^{z-1})(1) = O(h^z) + O(h^p)$$

holds for all $z \in \mathbb{C} \setminus \{0, -1, -2, \dots\}$.

Remark 4.3.1 a) We note that the condition for consistency can also be interpreted as

$$h^\alpha \sum_{j=0}^{\infty} \omega_j e^{-jh} = \frac{1}{\Gamma(\alpha)} \int_0^{\infty} t^{\alpha-1} e^{-t} dt + O(h^p), \quad \alpha > 0,$$

i.e. the convolution part of the fractional convolution quadrature yields an $O(h^p)$ approximation to the integral of the exponential function on the interval $(0, \infty)$.

b) The standardization at the point $x = 1$ in equation (4.45) is justified by

$$(4.46) \quad ({}_h E^\alpha t^{z-1})(x) = x^{\alpha+z-1} ({}_{h/x} E^\alpha t^{z-1})(1), \quad x > 0,$$

which can be deduced as follows: For $x > 0$ we have

$$J^\alpha x^{z-1} = \frac{\Gamma(z)}{\Gamma(z+\alpha)} x^{z-1+\alpha}$$

and

$$\begin{aligned} {}_h \Omega^\alpha x^{z-1} &= h^\alpha \sum_{j=0}^n \omega_{n-j} (jh)^{z-1} \quad (x = nh) \\ &= x^\alpha \left(\frac{h}{x}\right)^\alpha \sum_{j=0}^n \omega_{n-j} \left(\frac{j}{n}\right)^{z-1} = n^{-\alpha} \sum_{j=0}^n \omega_{n-j} \left(\frac{j}{n}\right)^{z-1} x^{z-1+\alpha}. \end{aligned}$$

Thus

$$\begin{aligned} {}_h E^\alpha (x^{z-1})(x) &= x^{z-1+\alpha} \left(n^{-\alpha} \sum_{j=0}^n \omega_{n-j} \left(\frac{j}{n}\right)^{z-1} - \frac{\Gamma(z)}{\Gamma(z+\alpha)} \right) \\ &= x^{z-1+\alpha} ({}_{h/x} E^\alpha t^{z-1})(1) \end{aligned}$$

c) It is important to point out that none of the above definitions of stability, consistency and convergence take the starting part ${}_h S^\alpha$ of the fractional convolution quadrature (4.44) into account. This fact will be fully explained later on in Theorem 4.3.12.

For the classical convolution quadrature Dahlquist had shown in [27] and [28] that convergence of a convolution quadrature is equivalent to stability and consistency (see also Chapter 2.2). The corresponding results for the fractional convolution quadrature were first stated by Lubich in [96], treated in more detail in the book of Brunner and van der Houwen [19] and later repeated and advanced by Nkarnang in [109]. We will restate and prove them here within our notations and based on already given results.

Theorem 4.3.1 *Let α be a non-integer number and r_1 and r_2 be rational functions. Then a fractional convolution quadrature ω , given by*

$$(4.47) \quad \omega(\zeta) = (r_1(\zeta))^\alpha r_2(\zeta)$$

is convergent of order p if and only if it is stable and consistent of order p .

Proof: We will divide the proof into smaller lemmata. Lemma 4.3.3 will prove that convergence of order p implies consistency of order p , Lemma 4.3.6 will show that stability also follows from convergence and finally in Lemma 4.3.10 we will see that stability and consistency of order p imply convergence of order p of a fractional convolution quadrature. A number of smaller auxiliary results for these three lemmata will also be needed and are thus stated on the following pages. \square

From now on we assume that the fractional convolution quadrature ω is given by (4.47).

Lemma 4.3.2 *Let $\alpha > 0$ and f and g be two continuous functions. Then*

$$(4.48) \quad {}_hE^\alpha(f * g) = {}_hE^\alpha f * g,$$

where $$ denotes the Laplace convolution (see Definition 3.1.3).*

Proof: The Riemann-Liouville integral operator can be understood as convolution, i.e.

$$(J^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t) dt = \left(\frac{x^{\alpha-1}}{\Gamma(\alpha)} * f \right)(x)$$

and thus by the associativity of the convolution operator it follows that

$$J^\alpha(f * g) = \frac{x^{\alpha-1}}{\Gamma(\alpha)} * (f * g) = \left(\frac{x^{\alpha-1}}{\Gamma(\alpha)} * f \right) * g = (J^\alpha f) * g$$

holds for the given functions f and g . Writing the convolution part of the fractional convolution quadrature ω as

$${}_h\Omega^\alpha f(x_n) = h^\alpha \sum_{j=0}^n \omega_j f(x_n - x_j)$$

we find that

$$(4.49) \quad \begin{aligned} ({}_h\Omega^\alpha(f * g))(x_n) &= h^\alpha \sum_{j=0}^n \omega_j (f * g)(x_n - x_j) \\ &= h^\alpha \sum_{j=0}^n \omega_j \int_0^{x_n - x_j} f(s) g(x_n - x_j - s) ds \\ &= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_0^{x_n - x_j} f(s) g(x_n - x_j - s) ds, \end{aligned}$$

where we used in the last step that

$$\lim_{x \rightarrow 0} (f * g)(x) = 0.$$

Furthermore,

$$\begin{aligned} ({}_h\Omega^\alpha f * g)(x_n) &= \int_0^{x_n} ({}_h\Omega^\alpha f)(t) g(x_n - t) dt \\ &= h^\alpha \int_0^{x_n} \sum_{0 \leq x_j \leq t} \omega_j f(t - x_j) g(x_n - t) dt \\ &= h^\alpha \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} \sum_{0 \leq x_j \leq t} \omega_j f(t - x_j) g(x_n - t) dt \\ &= h^\alpha \sum_{k=0}^{n-1} \sum_{j=0}^k \omega_j \int_{x_k}^{x_{k+1}} f(t - x_j) g(x_n - t) dt \\ &= h^\alpha \sum_{j=0}^{n-1} \omega_j \sum_{k=j}^{n-1} \int_{x_k}^{x_{k+1}} f(t - x_j) g(x_n - t) dt \\ &= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_{x_j}^{x_n} f(t - x_j) g(x_n - t) dt \\ &= h^\alpha \sum_{j=0}^{n-1} \omega_j \int_0^{x_n - x_j} f(s) g(x_n - x_j - s) ds \\ &= ({}_h\Omega^\alpha (f * g))(x_n) \quad \text{by (4.49).} \end{aligned}$$

With these results it follows directly that

$$\begin{aligned} {}_hE^\alpha(f * g) &= {}_h\Omega^\alpha(f * g) - J^\alpha(f * g) \\ &= {}_h\Omega^\alpha f * g - J^\alpha f * g \\ &= {}_hE^\alpha f * g. \end{aligned}$$

□

Lemma 4.3.3 *Let $\alpha > 0$ and ${}_hE^\alpha x^{k-1} = O(h^k) + O(h^p)$ for $k = 1, 2, 3, \dots$, then the fractional convolution quadrature ω is consistent of order p . In particular, convergence of order p implies consistency of order p .*

Proof: By Definition 4.3.2 2. for consistency of order p we need to show that $h^\alpha \omega(e^{-h}) = 1 + O(h^p)$. We will first prove that $\lim_{x \rightarrow \infty} e_h(x) = h^\alpha \omega(e^{-h}) - 1$ holds for an auxiliary function $e_h(x)$ and afterwards that $\lim_{x \rightarrow \infty} e_h(x) = O(h^p)$ holds, which will thus conclude our proof.

Let $u(t) = e^{t-x}$ be a function defined on the interval $[0, x]$. Then the convolution quadrature error of this function is given by

$$e_h(x) := ({}_hE^\alpha e^{t-x})(x) = h^\alpha \sum_{0 \leq jh \leq x} \omega_j e^{-jh} - (J^\alpha e^{t-x})(x)$$

$$= h^\alpha \sum_{0 \leq jh \leq x} \omega_j e^{-jh} - \frac{1}{\Gamma(\alpha)} \int_0^x s^{\alpha-1} e^{-s} ds.$$

Taking the limit $x \rightarrow \infty$ we get

$$(4.50) \quad \lim_{x \rightarrow \infty} e_h(x) = h^\alpha \omega(e^{-h}) - 1.$$

Using the identity

$$u(t) = J^m D^m u(t) + \sum_{j=0}^{m-1} \frac{u^{(j)}(0)}{j!} t^j, \quad m \in \mathbb{N}$$

and the fact that $u^{(m)}(t) = u(t)$ for all $m \in \mathbb{N}$ it follows that

$$\begin{aligned} e^{t-x} &= (J^m e^{s-x})(t) + \sum_{j=0}^{m-1} \frac{e^{-x}}{j!} t^j \\ &= \frac{1}{(m-1)!} (s^{m-1} * e^{s-x})(t) + e^{-x} \sum_{j=0}^{m-1} \frac{t^j}{j!}. \end{aligned}$$

Therefore, we can write the convolution quadrature error of $u(t)$ as

$$e_h(x) = e_h^1(x) + e_h^2(x),$$

where

$$e_h^1(x) := \frac{{}_h E^\alpha(t^{m-1} * e^{t-x})(x)}{(m-1)!} \quad \text{and} \quad e_h^2(x) := e^{-x} \sum_{j=0}^{m-1} \frac{1}{j!} ({}_h E^\alpha t^j)(x).$$

From result (4.48) of Lemma 4.3.2 follows:

$$\begin{aligned} (m-1)! e_h^1(t) &= {}_h E^\alpha(t^{m-1} * e^{t-x})(x) \\ &= ({}_h E^\alpha t^{m-1} * e^{t-x})(x) \\ &= \int_0^x e^{-s} ({}_h E^\alpha t^{m-1})(s) ds. \end{aligned}$$

Taking the limit $x \rightarrow \infty$ yields

$$\lim_{x \rightarrow \infty} e_h^1(x) = \frac{1}{(m-1)!} \int_0^\infty e^{-s} ({}_h E^\alpha t^{m-1})(s) ds.$$

From our remark (4.46) and the assumptions follows (with sufficiently large m , i.e. $m \geq p$) that

$$({}_h E^\alpha t^{m-1})(s) = s^{\alpha+m-1} ({}_{h/s} E^\alpha t^{m-1})(1) = O(s^{\alpha-1} h^p),$$

and thus

$$\lim_{x \rightarrow \infty} e_h^1(x) = O(h^p), \quad h \rightarrow 0.$$

From remark (4.46) also follows that $({}_hE^\alpha t^j)(x)$ has only polynomial growth as $x \rightarrow \infty$. Hence

$$\lim_{x \rightarrow \infty} e_h^2(x) = 0$$

and thus

$$\lim_{x \rightarrow \infty} e_h(x) = O(h^p)$$

from which consistency of order p follows immediately from (4.50). Obviously the definition of convergence is stricter than the required assumption in this lemma and thus convergence of order p implies consistency of order p . \square

Let us now consider the power series of the the generating function (4.47) from Theorem 4.3.1. We can write the function $\omega(\zeta)$ as

$$(4.51) \quad \omega(\zeta) = (1 - \zeta)^{-\mu} \tilde{\omega}(\zeta),$$

where μ is chosen such that $\tilde{\omega}(\zeta)$ is analytic at 1 and $\tilde{\omega}(1) \neq 0$. Consistency implies immediately $\mu = \alpha$ and $\tilde{\omega}(1) = 1$. Expanding ω at 1 yields:

$$(4.52) \quad \omega(\zeta) = (1 - \zeta)^{-\alpha} \left[c_0 + c_1(1 - \zeta) + \dots + c_{N-1}(1 - \zeta)^{N-1} \right] + (1 - \zeta)^N r(\zeta),$$

where $r(\zeta) := (1 - \zeta)^{-\alpha} \tilde{r}(\zeta)$ and $\tilde{r}(\zeta)$ is analytic at 1. Consistency can now be characterized in terms of the coefficients c_j in (4.52):

Lemma 4.3.4 *Let γ_j denote the coefficients of*

$$\sum_{j=0}^{\infty} \gamma_j (1 - \zeta)^j = \left(\frac{-\ln \zeta}{(1 - \zeta)} \right)^{-\alpha}.$$

Then the fractional convolution quadrature ω is consistent of order p if and only if the coefficients c_j in (4.52) satisfy $c_j = \gamma_j$ for $j = 0, 1, \dots, p-1$.

Proof: For consistency of order p we need to show that $h^\alpha \omega(e^{-h}) = 1 + O(h^p)$. From (4.51) follows

$$h^\alpha \omega(e^{-h}) = \left(\frac{h}{1 - e^{-h}} \right)^\alpha \tilde{\omega}(e^{-h})$$

which satisfies $1 + O(h^p)$ if and only if

$$\tilde{\omega}(e^{-h}) = \left(\frac{h}{1 - e^{-h}} \right)^{-\alpha} + O(h^p).$$

(in the above equation $O(h^{p-\alpha})$ would have been sufficient, but analyticity of $\tilde{\omega}$ implies $O(h^p)$). This holds if and only if

$$\tilde{\omega}(\zeta) = \left(\frac{-\ln \zeta}{1 - \zeta} \right)^{-\alpha} + O((1 - \zeta)^p).$$

\square

In the following lemmata we will use the fact that the binomial coefficients possess the asymptotic expansion:

$$(4.53) \quad (-1)^n \binom{-\alpha}{n} = \frac{n^{\alpha-1}}{\Gamma(\alpha)} [1 + a_1 n^{-1} + a_2 n^{-2} + \dots + a_{N-1} n^{-N+1} + O(n^{-N})],$$

where the coefficients a_j depend analytically on α . This result can be derived from the asymptotic behaviour of the quotient of two Gamma functions

$$\frac{\Gamma(n+r)}{\Gamma(n+s)} = n^{r-s} \sum_{j=0}^N \frac{b_j}{n^j} + n^{r-s} O(n^{-N-1}), \quad n \rightarrow \infty,$$

$$b_0 = 1, b_j = (-1)^j \frac{\Gamma(r-s+1)}{\Gamma(r-s)j!} B_j^{r-s+1}(r),$$

where

$$B_j^r(x) := \frac{d^j}{dt^j} \left[\left(\frac{1}{e^t - 1} \right)^r e^{xt} \right]_{t=0}$$

are the generalized Bernoulli-Polynomials [100, p. 19]. This result and the fact that

$$(-1)^n \binom{-\alpha}{n} = \frac{(-1)^n}{\Gamma(\alpha)} \frac{\Gamma(n+\alpha)}{\Gamma(n+1)}$$

imply that

$$a_j = (-1)^j \frac{\Gamma(1-\alpha+j)}{\Gamma(1-\alpha)j!} B_j^\alpha(\alpha), \quad j = 1, \dots, N-1$$

and thus that the a_i depend in fact analytically on α .

With this auxiliary result we can point out in which way the stability of a fractional convolution equation ω depends on the remainder of the expression (4.52):

Lemma 4.3.5 *The fractional convolution quadrature ω is stable if and only if the coefficients r_n of $r(\zeta)$ in (4.52) satisfy*

$$(4.54) \quad r_n = O(n^{\alpha-1}).$$

Proof: Let $r_n = O(n^{\alpha-1})$. For stability we have to show that $\omega_n = O(n^{\alpha-1})$. The convolution weights are given in equation (4.52) as

$$\omega_n = \sum_{j=0}^{N-1} (-1)^n \binom{-\alpha+j}{n} c_j + \sum_{k=0}^n (-1)^k \binom{-\alpha+N}{k} r_{n-k}.$$

Thus by (4.53) it follows that $\omega_n = O(n^{\alpha-1})$.

Conversely, let ω be stable. Then $\omega(\zeta)$ has no singularities in the interior of the unit disc and thus can be written as

$$(4.55) \quad \omega(\zeta) = u(\zeta) \left((\zeta-1)^{-\alpha} - \prod_{j=0}^m (\zeta - \zeta_j)^{-\alpha_j} \right),$$

where

$$|\zeta_j| = 1, \quad u(\zeta) \neq 0, \quad \alpha_j > 0, \quad \zeta_i \neq \zeta_j \quad \text{for } i, j = 1, \dots, m$$

and $u(\zeta)$ is analytic in a neighbourhood of $|\zeta| \leq 1$. A partial fraction decomposition of $\omega(\zeta)$ yields

$$\omega(\zeta) = (\zeta - 1)^{-\alpha} u(\zeta) + \sum_{j=1}^m (\zeta - \zeta_j)^{-\alpha_j} p_j(\zeta - \zeta_j) + q(\zeta),$$

where the p_j are polynomials satisfying $p_j(0) \neq 0$ and $q(\zeta)$ is analytic in the interior of the unit disc and sufficiently differentiable on the unit circle $|\zeta| = 1$. From (4.53) follows

$$(4.56) \quad \omega_n = O(n^{\alpha-1}) \quad \text{if and only if} \quad \alpha_j \leq \alpha, \quad j = 1, \dots, m.$$

Correspondingly, $r(\zeta)$ can be represented as

$$r(\zeta) = (\zeta - 1)^{-\alpha} \tilde{u}(\zeta) + \sum_{j=1}^m (\zeta - \zeta_j)^{-\alpha_j} \tilde{p}_j(\zeta - \zeta_j) + \tilde{q}(\zeta)$$

with \tilde{u} , \tilde{p}_j and \tilde{q} are linked to $\tilde{\omega}$ as u, p_j and q to ω . Thus $r_n = O(n^{\alpha-1})$ holds. \square

Lemma 4.3.6 *The fractional convolution quadrature ω is stable of order p if it is convergent of order p .*

Proof: Convergence of ω implies $({}_h E^\alpha x^{z-1})(1) = O(h^z) + O(h^p)$. By Lemma 4.3.3 this implies also consistency of ω . We can therefore write $\omega(\zeta)$ with $N = 1$ in (4.52) as

$$\begin{aligned} \omega(\zeta) &= (1 - \zeta)^{-\alpha} + (1 - \zeta)r(\zeta) \\ \Leftrightarrow \frac{\omega(\zeta)}{1 - \zeta} &= (1 - \zeta)^{-\alpha-1} + r(\zeta), \end{aligned}$$

and thus

$$(-1)^n \binom{-\alpha-1}{n} + r_n$$

is the n th coefficient of $\omega(\zeta)/(1 - \zeta)$. On the other hand

$$\begin{aligned} \frac{\omega(\zeta)}{1 - \zeta} &= \omega(\zeta) \frac{1}{1 - \zeta} = \left(\sum_{j=0}^{\infty} \omega_j \zeta^j \right) \left(\sum_{k=0}^{\infty} \zeta^k \right) \\ &= \sum_{j=0}^{\infty} \sum_{k=0}^j \omega_{j-k} \zeta^j. \end{aligned}$$

Therefore, we can conclude

$$\sum_{k=0}^n \omega_{n-k} = (-1)^n \binom{-\alpha-1}{n} + r_n.$$

We now consider the convolution quadrature error

$$\begin{aligned}({}_hE^\alpha 1)(1) &= h^\alpha \sum_{j=0}^n \omega_{n-j} - \frac{1}{\Gamma(\alpha+1)}, \quad (hn = 1) \\ &= h^\alpha \left[(-1)^n \binom{-\alpha-1}{n} \right] + h^\alpha r_n - \frac{1}{\Gamma(\alpha+1)}.\end{aligned}$$

With (4.53) follows

$$\begin{aligned}({}_hE^\alpha 1)(1) &= h^\alpha \left[\frac{n^\alpha}{\Gamma(\alpha+1)} + O(n^{\alpha-1}) \right] + h^\alpha r_n - \frac{1}{\Gamma(\alpha+1)} \\ &= O(h) + h^\alpha r_n.\end{aligned}$$

Thus $({}_hE^\alpha 1)(1) = O(h)$ if and only if $r_n = O(n^{\alpha-1})$. \square

We still need to show that stability and consistency imply convergence. Before we can accomplish that we need to state some results on the structure of the error of the fractional convolution quadrature ω . We will use the following auxiliary result on the convolution of two sequences $u_n = O(n^\mu)$ and $v_n = O(n^\nu)$ with $\nu < \min\{-1, \mu - 1\}$: From

$$\left| \sum_{j=0}^n u_{n-j} v_j \right| \leq |u_n v_0| + |u_0 v_n| + M n^\mu \sum_{j=0}^{n-1} \left(1 - \frac{j}{n} \right)^\mu j^\nu$$

and

$$\left(1 - \frac{j}{n} \right)^\mu \leq \begin{cases} 1 & \text{if } \mu \geq 0, \\ (j+1)^{-\mu} & \text{if } \mu < 0 \end{cases}$$

for $1 \leq j \leq n-1$ follows that

$$(4.57) \quad \sum_{j=0}^n u_{n-j} v_j = O(n^\mu).$$

With this auxiliary result we can prove a first result on the quadrature error of the fractional convolution quadrature ω :

Lemma 4.3.7 *Let $\alpha, z > 0$ and the fractional convolution quadrature ω be stable. Then the convolution quadrature error of t^{z-1} has an asymptotic expansion of the form*

$$(4.58) \quad ({}_hE^\alpha t^{z-1})(1) = e_0 + e_1 h + \dots + e_{N-1} h^{N-1} + O(h^N) + O(h^z).$$

Proof: We consider the power series

$$b(\zeta) := \sum_{n=1}^{\infty} n^{z-1} \zeta^n.$$

From (4.53) we obtain an asymptotic expansion:

$$n^{z-1} = \sum_{k=0}^{N-1} b_k (-1)^k \binom{-z+k}{n} + O(n^{z-1-N}).$$

Therefore, we can write

$$(4.59) \quad b(\zeta) = \sum_{k=0}^{N-1} b_k (1 - \zeta)^{-z+N-1} + s(\zeta),$$

where the coefficients s_n of $s(\zeta)$ satisfy

$$(4.60) \quad s_n = O(n^{z-1-N}).$$

At this point we need to study the expression

$$h^\alpha \sum_{j=1}^n \omega_{n-j} (jh)^{z-1}, \quad (hn = 1).$$

If we define

$$y(\zeta) := \omega(\zeta)b(\zeta) = \sum_{k=0}^{\infty} y_k \zeta^k$$

we immediately get that $y_n = \sum_{j=1}^n \omega_{n-j} j^{z-1}$, which by inserting in (4.59) and (4.52) yields

$$\begin{aligned} y(\zeta) &= \left(\sum_{j=0}^{N-1} c_j (1 - \zeta)^{j-\alpha} + (1 - \zeta)^N r(\zeta) \right) \left(\sum_{k=0}^{N-1} b_k (1 - \zeta)^{-z+N-1} + s(\zeta) \right) \\ &= \sum_{j=0}^{2N-2} \left(\sum_{k=0}^j b_{i-k} c_j \right) (1 - \zeta)^{-(\alpha+z)+j} + \omega(\zeta)s(\zeta) + [b(\zeta) - s(\zeta)](1 - \zeta)^N r(\zeta). \end{aligned}$$

Let now N be such that $z - 1 - N < \min\{-1, \alpha - 2\}$, then

$$\begin{aligned} \omega(\zeta)s(\zeta) &= \left(\sum_{j=0}^{\infty} \omega_j \right) \left(\sum_{k=0}^{\infty} s_k \right) \\ &= \sum_{j=0}^{\infty} \left(\sum_{k=0}^j \omega_{j-k} s_k \right) \zeta^j. \end{aligned}$$

Since ω is stable it follows from (4.60) and the result (4.57) that the coefficients of $\omega(\zeta)s(\zeta)$ are $O(n^{\alpha-1})$. Furthermore, the coefficients of

$$[b(\zeta) - s(\zeta)](1 - \zeta)^N r(\zeta) = [b_0(1 - \zeta)^{-\beta+n} + \dots + b_{N-1}(1 - \zeta)^{-\beta+2N-1}]r(\zeta)$$

are $O(n^{\alpha-1})$ by (4.53), (4.54), (4.57) and (4.60). With (4.53) we also get

$$y_n = e_0 n^{\alpha+z-1} + e_1 n^{(\alpha+z-1)-1} + \dots + e_N n^{(\alpha+z-1)-N} + O(n^{\alpha-1}).$$

Finally (4.58) follows with

$$({}_h E^\alpha t^{z-1})(1) = h^{\alpha+z-1} y_n - \frac{\Gamma(z)}{\Gamma(\alpha+z)}, \quad (hn = 1).$$

□

Lemma 4.3.8 *Let $\alpha > 0$ and $({}_hE^\alpha t^{p-1})(1) = O(h^p)$. Then*

$$({}_hE^\alpha t^{q-1})(1) = O(h^p), \quad \text{for all } q > p.$$

Proof: Let $q = p + \mu$. We can express t^{q-1} as convolution

$$t^{q-1} = \frac{\Gamma(p+\mu)}{\Gamma(p)\Gamma(\mu)} t^{p-1} * t^{\mu-1}$$

and by remark (4.46) we get

$$\begin{aligned} ({}_hE^\alpha t^{p-1})(x) &= x^{\alpha+p-1} ({}_{h/x}E^\alpha t^{p-1})(1) \\ &= x^{\alpha+p-1} \left(\left(\frac{h}{x} \right)^p \right) \\ &= O(x^{\alpha-1} h^p). \end{aligned}$$

On the other hand (4.48) yields

$${}_hE^\alpha (t^{p-1} * t^{\mu-1})(1) = ({}_hE^\alpha t^{p-1} * t^{\mu-1})(1) = O(h^p)$$

and thus also

$$({}_hE^\alpha t^{q-1})(1) = O(h^p).$$

□

Lemma 4.3.9 *Let $\alpha > 0$ and let ω be a stable fractional convolution quadrature. Then there exist numbers $\gamma_0, \gamma_1, \gamma_2, \dots$ independent of the generating function $\omega(\zeta)$ such that the following equivalence holds:*

$$(4.61) \quad ({}_hE^\alpha t^{q-1})(1) = O(h^q) \quad \text{for } q = 1, 2, \dots, p$$

if and only if the coefficients c_i in (4.52) satisfy

$$(4.62) \quad c_i = \gamma_i \quad \text{for } i = 0, 1, \dots, p-1.$$

Proof: The proof proceeds by induction on p . Trivially the statement holds true for $p = 0$. Assuming that the statement already has been proven up to order p , we need to show that it holds true for $p + 1$. Under the assumption that (4.61) or (4.62) holds, it suffices to prove that c_p can be uniquely chosen such that

$$({}_hE^\alpha t^p)(1) = O(h^{p+1}).$$

By (4.61) and Lemma 4.3.8 follows

$$(4.63) \quad ({}_hE^\alpha t^p)(1) = O(h^p).$$

In order to show under which conditions we get $O(h^{p+1})$ we note that any given integer n to the power of p can be expressed as

$$n^p = \sum_{k=1}^{p+1} a_k \binom{n+k-1}{n} = \sum_{k=0}^{p+1} a_k (-1)^n \binom{-k}{n}$$

with suitable coefficients a_i . From this expression with $hn = 1$ we gain that

$$({}_h\Omega^\alpha t^p)(1) = h^\alpha \sum_{j=0}^n \omega_j (n-j)^p h^p = h^{p+\alpha} \sum_{k=1}^{p+1} a_k \sum_{j=0}^n \omega_j (-1)^{n-j} \binom{-k}{n-j}.$$

On the other hand the inner sum is the n th coefficient of

$$\begin{aligned} \frac{\omega(\zeta)}{(1-\zeta)^k} &= \gamma_0(1-\zeta)^{-\alpha-k} + \dots + \gamma_{p-1}(1-\zeta)^{-\alpha+p-1-k} \\ &\quad + c_p(1-\zeta)^{-\alpha+p-k} + (1-\zeta)^{p+1-k} r(\zeta). \end{aligned}$$

With (4.53), (4.54) and (4.63) we obtain

$$({}_hE^\alpha t^p)(1) = \frac{c_p - \gamma_p}{\Gamma(\alpha+1)} h^p + O(h^{p+1}).$$

Hence (4.61) holds for $p+1$ if and only if $c_p = \gamma_p$. \square

We may also note that by Lemma 4.3.3 equation (4.61) also implies consistency of the fractional convolution quadrature used in Lemma 4.3.9 given that (4.62) holds. Thus we can now easily prove

Lemma 4.3.10 *Let $\alpha > 0$ and let the fractional convolution quadrature ω be stable and consistent of order p , then ω is convergent of order p .*

Proof: First we note that the numbers γ_i of Lemma 4.3.9 and Lemma 4.3.4 are identical since ω is assumed to be consistent. Moreover, because of the stability of ω we get from Lemma 4.3.7 and Lemma 4.3.8 for $z > p$

$$e_k(\alpha, z, \gamma_0, \dots, \gamma_j) = 0, \quad k = 0, \dots, p-1.$$

At last, by Lemma 4.3.4 consistency of order p implies

$$e_i = \gamma_i \quad i = 0, \dots, p-1,$$

so that

$$({}_hE^\alpha x^{z-1})(1) = O(h^z) + O(h^p)$$

holds for all $z \in \mathbb{C} \setminus \{0, -1, -2, \dots\}$ and thus ω is convergent of order p . \square

With this lemma we have successfully proven Theorem 4.3.1. Furthermore, by choosing $\alpha = 1$ in the fractional convolution quadrature (4.47) we have in essence reproduced Dahlquist's convergence theorem for linear multistep methods [27, 28].

There is another important result by Dahlquist in [29], which we want to transfer to the fractional case: If we take $({}_hJf)(x)$ as solution of a linear multistep method (σ, ρ) applied to the problem $y' = f$, $y(0) = 0$ as described in Lemma 2.2.6, then Dahlquist showed that the repeated method $({}_hJ^k f)(x) = ({}_hJ \dots {}_hJf)(x)$, $k \in \mathbb{N}$ can be written as convolution quadrature, where the convolution weights ω_n are coefficients of the generating function $\omega(\zeta)^k$. This method can be interpreted as k th power of the multistep method. In the following theorem we are interested in a similar approach for the case that k is not an integer, i.e. we are interested in the α th power of a linear multistep method, with $\alpha \in \mathbb{R}$.

Theorem 4.3.11 *Let (σ, ρ) denote an implicit classical linear multistep method which is stable and consistent of order p and assume that all zeros of $\sigma(\zeta)$ lie inside or on the unit disc. Furthermore, let ω be the generating function of the linear multistep method. If we define the generating function $\omega^\alpha(\zeta)$ by*

$$(4.64) \quad \omega^\alpha(\zeta) = (\omega(\zeta))^\alpha,$$

the fractional convolution quadrature ω^α is convergent of order p to J^α .

Proof: Because of Theorem 4.3.1 we only need to show that ω^α is consistent and stable. Consistency immediately follows from the consistency of order p of the underlying multistep method, i.e.

$$h\omega(e^{-h}) = 1 + O(h^p).$$

Taking this relation to the power α yields

$$h^\alpha \omega^\alpha(e^{-h}) = 1 + O(h^p).$$

so that ω^α is consistent of order p to J^α . To prove stability of the method, we note that under the given assumptions on (σ, ρ) we can write

$$\omega(\zeta) = \frac{\sigma(\zeta^{-1})}{\rho(\zeta^{-1})} = \prod_{j=0}^r (1 - \zeta_j \zeta)^{-1} v(\zeta),$$

where $v(\zeta)$ is analytic and without zeros in a neighbourhood of $|\zeta| \leq 1$, and ζ_j are the zeros of $\rho(\zeta)$ on the unit circle. Thus

$$\omega^\alpha(\zeta) = \prod_{j=0}^r (1 - \zeta_j \zeta)^{-\alpha} u(\zeta),$$

where $u(\zeta) = v(\zeta)^\alpha$ is analytic in a neighbourhood of $|\zeta| \leq 1$. With (4.55) and (4.56) we get

$$\omega_n^\alpha = O(n^{\alpha-1})$$

so that ω^α is stable. □

We come back to the earlier mentioned fact, that in the Definition 4.3.2 the stability, consistency and convergence of a fractional convolution quadrature were defined without the use of the starting part in (4.44). If we consider a fractional convolution quadrature as defined in (4.44), which converges with order p to J^α , we will always be able to find a set of starting weights, so that for a sufficiently well behaved function f the fractional convolution quadrature error, i.e. ${}_h J^\alpha f - J^\alpha f$, is also of order p . The following two lemmata define what we understand under a sufficiently well behaved function f and show how we obtain the set of starting weights. They are generalizations of Theorem 2.4 in [96] and Theorem 6.1.4 in [19], which were given in the way we state them here in [109].

Theorem 4.3.12 *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad \alpha > 0.$$

Furthermore, let

$$(4.65) \quad f(x) := \sum_{j=0}^L x^{z_j} v_j(x), \quad 0 \leq z_j \leq p-1, \quad v_j \in C^p[0, X], \quad j = 0, \dots, L$$

and

$$(4.66) \quad A_j := \{\gamma = k + z_j | k \in \mathbb{N}_0, \gamma \leq p-1\}, \quad A := \bigcup_{j=0}^L A_j,$$

and $s_j := \text{card} A_j - 1$, $s := \text{card} A - 1$. If we define the starting weights w_{nj} by the linear system

$$(4.67) \quad \sum_{j=0}^s w_{nj} j^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+\alpha+1)} n^{\gamma+\alpha} - \sum_{j=0}^n \omega_{n-j} j^\gamma, \quad \gamma \in A,$$

then the following statements hold:

1. $w_{nj} = O(n^{\alpha-1})$, $j = 0, \dots, s$,
2. ${}_h J^\alpha f(x) - J^\alpha f(x) = O(h^{p-\varepsilon})$, with some $0 \leq \varepsilon < 1$ uniformly for all fixed $x_n = nh =: x \in [0, X]$.

Proof: 1. Because the convolution quadrature ω is convergent, we immediately get from Theorem 4.3.11

$$({}_h E^\alpha x^{z-1})(1) = O(h^z) + O(h^p), \quad \text{for all } z > 0.$$

The system (4.67) is motivated by

$$\begin{aligned} ({}_h E^\alpha x^\gamma)(1) &= h^\alpha \sum_{j=0}^n \omega_{n-j} (jh)^\gamma - \frac{1}{\Gamma(\alpha)} \int_0^1 (1-t)^{\alpha-1} t^\gamma dt \\ &= h^{\alpha+\gamma} \sum_{j=0}^n \omega_{n-j} j^\gamma - \frac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} \\ &= h^{\alpha+\gamma} \left[\sum_{j=0}^n \omega_{n-j} j^\gamma - \frac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} n^{\alpha+\gamma} \right] \quad (nh = 1) \\ &= h^{\alpha+\gamma} \sum_{j=0}^s w_{nj} j^\gamma, \end{aligned}$$

i.e. the starting weights w_{nj} in (4.67) are chosen such that

$$(4.68) \quad ({}_h J^\alpha - J^\alpha) x^{i+z_j} = 0, \quad \text{for all } i \in \{0, \dots, s_j\}, \quad \text{and } j \in \{1, \dots, L\}.$$

In addition for $\gamma \in A$ we get

$$\begin{aligned}
 \sum_{j=0}^s w_{nj} j^\gamma &= \frac{1}{h^{\alpha+\gamma}} ({}_h E^\alpha x^\gamma)(1) \\
 &= \frac{1}{h^{\alpha+\gamma}} (O(h^{\gamma+1}) + O(h^p)) \\
 &= O(h^{-\alpha+1}) + O(h^{p-\alpha-\gamma}) \quad (nh = 1) \\
 &= O(n^{\alpha-1})
 \end{aligned}$$

and thus

$$w_{nj} = O(n^{\alpha-1}), \quad j = 0, \dots, s.$$

2. A Maclaurin expansion of v_j yields

$$v_j(x) = \sum_{k=0}^{s_j} \frac{v_j^{(k)}(0)}{k!} x^k + \frac{x^{s_j+1}}{(s_j+1)!} v_j^{(s_j+1)}(\xi_j), \quad \xi_j \in (0, x).$$

Thus we get for $f(x)$:

$$f(x) = \sum_{j=0}^L \sum_{k=0}^{s_j} \frac{v_j^{(k)}(0)}{k!} x^{z_j+k} + \sum_{j=0}^L \frac{x^{s_j+z_j+1}}{(s_j+1)!} v_j^{(s_j+1)}(\xi_j), \quad \xi_j \in (0, x).$$

Furthermore, we have for $m \in \mathbb{N}$ with $m > p - z_j - 1$:

$$\begin{aligned}
 ({}_h J^\alpha - J^\alpha) x^{m+z_j} &= ({}_h E^\alpha t^{m+z_j})(x) + h^\alpha \sum_{k=0}^s w_{nk} (kh)^{m+z_j} \\
 &= x^{\alpha+m+z_j} ({}_h E^\alpha t^{m+z_j})(1) + h^{\alpha+m+z_j} \sum_{k=0}^s w_{nk} k^{m+z_j} \\
 &= x^{\alpha+m+z_j} \left(({}_h E^\alpha t^{m+z_j})(1) + \left(\frac{h}{x}\right)^{\alpha+m+z_j} \sum_{k=0}^s w_{nk} k^{m+z_j} \right) \\
 &= x^{\alpha+m+z_j} \left[O\left(\left(\frac{h}{x}\right)^{m+z_j+1}\right) + O\left(\left(\frac{h}{x}\right)^p\right) + O\left(\left(\frac{h}{x}\right)^{m+z_j+1}\right) \right] \\
 &= O(x^{\alpha+m+z_j-p} h^p).
 \end{aligned}$$

Thus we get overall (with $s_j + 1 \geq m$)

$$\begin{aligned}
 ({}_h J^\alpha - J^\alpha) f(x) &= \sum_{j=0}^L \sum_{k=0}^{s_j} \frac{v_j^{(k)}(0)}{k!} ({}_h J^\alpha - J^\alpha) x^{z_j+k} + \sum_{j=0}^L \frac{v_j^{(s_j+1)}(\xi_j)}{(s_j+1)!} ({}_h J^\alpha - J^\alpha) x^{s_j+z_j+1} \\
 &= \sum_{j=0}^L O(x^{\alpha+s_j+z_j-p+1} h^p).
 \end{aligned}$$

Let $T := \{j | \alpha + s_j + z_j - p + 1 \leq 0\}$. If $j \notin T$ it follows that

$$0 \leq x^{\alpha+s_j+z_j-p+1} \leq X^{\alpha+s_j+z_j-p+1}$$

and thus $x^{\alpha+s_j+z_j-p+1}$ is bounded. Hence $O(x^{\alpha+s_j+z_j-p+1}h^p) = O(h^p)$. If on the other hand $j \in T$ we get with $x = nh$ and $n^{\alpha+s_j+z_j-p+1} \leq 1$ that

$$O(x^{\alpha+s_j+z_j-p+1}h^p) = O(n^{\alpha+s_j+z_j-p+1}h^{\alpha+s_j+z_j+1}) = O(h^{\alpha+s_j+z_j+1}).$$

Therefore, we define

$$(4.69) \quad \varepsilon := \begin{cases} 0 & \text{if } T = \emptyset \\ \max_{j \in T} \{p - \alpha - s_j - z_j - 1\} & \text{if } T \neq \emptyset. \end{cases}$$

Obviously $0 \leq \varepsilon < 1$ and from

$$\alpha + s_j + z_j + 1 = p - (p - \alpha - s_j - z_j - 1) \geq p - \varepsilon, \quad \text{for all } j \in T$$

we get the error

$${}_hJ^\alpha f(x) - J^\alpha f(x) = O(h^{p-\varepsilon}).$$

□

With this result we can easily see, why Theorem 4.1.30 holds. There we stated that the finite Grünwald-Letnikov operator gives a first order approximation to the fractional derivative of $f(x)$ if and only if $f(x)$ is zero at the origin: First we note that the equation (4.21) defining the finite Grünwald-Letnikov operator is equivalent to the convolution part of the fractional backward difference method of order $p = 1$ (see also Chapter 5.1.1). Thus we know that the requirements on $\omega(\zeta)$ of Theorem 4.3.12 are met. By the assumptions of $f(x)$ in Theorem 4.1.30 we furthermore know that $z_1 = 0$ in equation (4.65) of Theorem 4.3.12 and thus $s = 0$ and $A = \{0\}$. Accordingly we get one starting weight, given by formula (4.67) which will be multiplied in the fractional convolution quadrature with the value of $f(x)$ at the origin. Therefore, Theorem 4.1.30 is given directly.

The next theorem states a result on the set of starting weights, if the function $f(x)$, to be approximated by a fractional convolution quadrature, possesses a singularity at the origin.

Theorem 4.3.13 *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad \alpha > 0.$$

Furthermore, let

$$(4.70) \quad f(x) := \sum_{j=0}^L x^{r_j-1} v_j(x), \quad 0 \leq r_j \leq p, \quad v_j \in C^p[0, X], \quad j = 0, \dots, L$$

and

$$(4.71) \quad A_j := \{\gamma = k + r_j | k \in \mathbb{N}_0, \gamma \leq p\}, \quad A := \bigcup_{j=0}^L A_j,$$

and $s_j := \text{card} A_j - 1$, $s := \text{card} A - 1$. If we define the starting weights w_{nj} by the linear system

$$(4.72) \quad \sum_{j=0}^s w_{nj} j^\gamma = \frac{\Gamma(\gamma)}{\Gamma(\gamma + \alpha)} n^{\gamma + \alpha + 1} - \sum_{j=0}^n \omega_{n-j} j^{\gamma-1}, \quad \gamma \in A,$$

then the following statements hold:

1. $w_{nj} = O(n^{\alpha-1})$, $j = 0, \dots, s$,
2. ${}_h J^\alpha f(x) - J^\alpha f(x) = O(h^{p-\varepsilon})$, with some $0 \leq \varepsilon < 1$ uniformly for all fixed $x_n = nh =: x \in [0, X]$.

Proof: The proof follows the same ideas as the proof of Theorem 4.3.12. The value of ε in this case is

$$\varepsilon := \begin{cases} 0 & \text{if } T = \emptyset \\ \max_{j \in T} \{p - s_j - r_j - \alpha\} & \text{if } T \neq \emptyset. \end{cases}$$

□

We deduce the following corollary from Theorems 4.3.12 and 4.3.13:

Corollary 4.3.14 *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad \alpha > 0.$$

If we define the starting weights w_{nj} by the linear system

$$(4.73) \quad \sum_{j=0}^s w_{nj} j^{z+r-1} = \frac{\Gamma(z+r)}{\Gamma(z+r+\alpha)} n^{z+r+\alpha-1} - \sum_{j=0}^n \omega_{n-j} j^{z+r-1}, \quad z = 1, \dots, s,$$

where $s \in \mathbb{N}$ is chosen such that

$$(4.74) \quad s + r \leq p \leq s + r + 1.$$

Then the following statements hold:

1. $w_{nj} = O(n^{\alpha-1})$, $j = 0, \dots, s$.
2. For $f(x) = x^{r-1}v(x)$, $v \in C^p[0, X]$, $r = \tilde{r} + k$, $\tilde{r} \in [0, 1)$, $k \in \mathbb{N}_0$ the convolution quadrature error satisfies

$$(4.75) \quad {}_h J^\alpha f(x) - J^\alpha f(x) = O(x^{\alpha-\tilde{r}} h^p)$$

uniformly for all fixed $x_n = nh =: x \in [0, X]$.

The last results stated that we will always find a set of starting weights so that the error of the fractional convolution quadrature behaves as it does in the case of classical convolution quadratures.

We are now going to extend Theorem 4.3.12 to Volterra-Abel integral equations of the second kind, i.e. we will be interested in convolution quadrature for equations of the form (see also Definition 4.2.2)

$$(4.76) \quad y(x) = f(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} K(x, t, y(t)) dt, \quad x \in [0, X], \quad \alpha > 0$$

where the kernel $K(x, t, y(t))$ is a bounded (and usually smooth) function. From Theorem 4.2.3 we know that fractional order differential equations can be transferred to Volterra integral equations of the form (4.76), where the function $f(x)$ is defined by the initial condition(s) and the kernel K is the right-hand side of the fractional order differential equation. Thus by construction a fractional convolution quadrature for the equation (4.76) will give results for fractional order differential equations as well. The following results are based on an article by Lubich [95]:

From Corollary 4.2.8 we know that if the function F with $f(x) = F(x, x^\alpha)$ and the kernel $K(x, t, y)$ in (4.43) are sufficiently differentiable the solution $y(x)$ is unique on its nonempty existence interval (assumed to contain the whole interval $[0, X]$) and can be written as

$$(4.77) \quad y(x) = Y(x, x^\alpha)$$

for some sufficiently differentiable function $Y(x_1, x_2)$. We now can state the following result:

Theorem 4.3.15 *Let (σ, ρ) be a convergent implicit linear multistep method of order $p \geq 1$ and let all zeros of $\sigma(\zeta)$ lie inside or on the unit disc and*

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha, \quad 0 < \alpha < 1.$$

Furthermore, set

$$(4.78) \quad A = \{\gamma = k + j\alpha; k, j \in \mathbb{N}_0, \gamma \leq p-1\}, \quad \text{card} A = s+1$$

and define

$$(4.79) \quad y_n = f(x_n) + h^\alpha \sum_{j=0}^n \omega_{n-j} K(x_n, x_j, y(x_j)) + h^\alpha \sum_{j=0}^s w_{n,j} K(x_n, x_j, y(x_j))$$

as discretization of the Volterra-Abel integral equation (4.76), where the convolution weights ω_k are given by the generating function $\omega^\alpha(\zeta)$ and the starting weights are constructed by the linear equation system

$$(4.80) \quad \sum_{j=0}^s w_{n,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma+\alpha)} n^{\alpha+\gamma} - \sum_{j=1}^n \omega_{n-j} j^\gamma, \quad \gamma \in A.$$

Then $w_{n,j} = O(n^{\alpha-1})$ and the numerical solution y_n satisfies

$$(4.81) \quad \max_{0 \leq n \leq N} |y_n - y(x_n)| = O(h^{p-\varepsilon}),$$

with some $0 \leq \varepsilon < 1 - \alpha$. In particular $\varepsilon = 0$ if $\alpha = q/(q+1)$ with $q \in \mathbb{N}$.

Remark 4.3.2 a) The notation of Theorem 4.3.15, in particular the definition of A , differs slightly from the one of Theorem 4.3.13. We used this notation for its easier use in the upcoming chapter on numerical methods, where we will directly use the equation system (4.80) for the starting weights.

The connection of the set A defined in (4.66) and (4.78) can be produced as follows: If $y(x)$ is sufficiently differentiable we gain from Corollary 4.2.8:

$$\begin{aligned}
 y(x) &= Y(x, x^\alpha) = \sum_{k=0}^{L_1} \sum_{j=0}^{L_2} f_{k,j} x^{k+j\alpha} + O(x^p) \\
 &= \sum_{k=0}^{L_1} f_k x^k \sum_{j=0}^{L_2} g_j x^{j\alpha} + O(x^p) \\
 &= \sum_{k=0}^{L_1} f_k x^k \sum_{j=0}^{L_2} g_j x^{z_j} + O(x^p), \quad z_j = j\alpha \\
 &= \sum_{j=0}^L v_j(x) x^{z_j},
 \end{aligned}$$

where $v_j(x)$ are polynomials of degree p for $j = 1, \dots, L$ and $v_0(x) \in C^p([0, X])$. Equivalently we then could define

$$\begin{aligned}
 A_j &:= \{\gamma = k + z_j | k \in \mathbb{N}_0, \gamma \leq p-1\} \\
 &= \{\gamma = k + j\alpha | k \in \mathbb{N}_0, \gamma \leq p-1\}
 \end{aligned}$$

and

$$A := \bigcup_{j=0}^L A_j,$$

where $s_j := \text{card} A_j - 1$, $s := \text{card} A - 1$.

b) If we apply the fractional convolution quadrature (4.44) directly to the Volterra-Abel integral equation (4.76) we get

$$\begin{aligned}
 (4.82) \quad y(x_n) &= f(x_n) + h^\alpha \sum_{j=0}^n \omega_{n-j} K(x_n, x_j, y(x_j)) \\
 &\quad + h^\alpha \sum_{j=0}^s w_{n,j} K(x_n, x_j, y(x_j)) + E_n^\alpha[\phi_n]
 \end{aligned}$$

where

$$E_n^\alpha[\phi_n] := \int_0^{x_n} (x_n - t)^{\alpha-1} \phi_n(t) dt - h^\alpha \sum_{j=0}^n \omega_{n-j} \phi_n(x_j) - h^\alpha \sum_{j=0}^s w_{n,j} \phi_n(x_j)$$

and $\phi_n(t) := K(x_n, t, y(t))$. We note especially, that representation (4.82) is not an approximation of $y(x_n)$ but its exact solution. Thus the term $E_n^\alpha[\phi_n]$ describes the error of the fractional convolution quadrature (4.79) for the Volterra-Abel integral equation (4.76).

A proof of Theorem 4.3.15 is given in [95] using discretized operational calculus [99]. We will state here a proof which uses representation (4.82) and is based on a proof given in the book by Brunner and van der Houwen [19, Thm. 6.1.6.]. Before we can prove Theorem 4.3.15 we need to state an auxiliary result:

Lemma 4.3.16 *Let $z_n \geq 0$ for $n = 0, 1, \dots, N$ and suppose that the sequence $\{z_n\}$ obeys the inequality*

$$(4.83) \quad z_n \leq h^\alpha C_0 \sum_{j=0}^{n-1} (n-j)^{\alpha-1} z_j + C_1, \quad n = 0, 1, \dots, N$$

with $0 < \alpha < 1$, $C_1 \geq 0$ and $C_0 > 0$ independent of $h > 0$. Then

$$(4.84) \quad z_n \leq C_1 E_\alpha(C_0 \Gamma(\alpha)(nh)^\alpha), \quad n = 0, 1, \dots, N$$

where E_α denotes the Mittag-Leffler function.

Proof: A proof of this lemma can be found e.g. in [45, Thm. 6.1] □

Proof: (of Theorem 4.3.15) The ω_{nj} in (4.80) are well defined, independent of h and of magnitude $O(n^{\alpha-1})$ (the last statement follows immediately from the proof of Theorem 4.3.12). For ease of notation we assume that the kernel is linear, i.e. $K(x, t, y(t)) = K(x, t)y(t)$, and define

$$e_n = y(x_n) - y_n.$$

Then, with equation (4.82), e_n can be written as

$$(4.85) \quad e_n = h^\alpha \sum_{j=0}^s (\omega_{n-j} + w_{n,j}) K(x_n, x_j) e_j + h^\alpha \sum_{j=s+1}^n \omega_{n-j} K(x_n, x_j) e_j + E_n^\alpha[\phi_n]$$

for $n = 1, \dots, N$ with $e_0 = 0$. We divide our further investigation of equation (4.85) into two different cases:

Case I ($1 \leq n \leq s$): In this case the equation (4.85) represents a nonsingular linear equation system in \mathbb{R}^s and thus the order of the starting errors e_1, \dots, e_s are given by the order of the quadrature errors $E_n^\alpha[\phi_n]$, $n = 1, \dots, s$, defining the right-hand side of the equation system.

Case II ($s+1 \leq n \leq N$): Rewriting equation (4.85) yields:

$$\begin{aligned} (1 - h^\alpha \omega_0 K(x_n, x_n)) e_n &= h^\alpha \sum_{j=0}^s (\omega_{n-j} + w_{n,j}) K(x_n, x_j) e_j \\ &\quad + h^\alpha \sum_{j=s+1}^{n-1} \omega_{n-j} K(x_n, x_j) e_j + E_n^\alpha[\phi_n]. \end{aligned}$$

From the behaviour of the starting and convolution weights we get

$$|\omega_{n-j}| \leq c_1 (n-j)^{\alpha-1} \quad \text{and} \quad |w_{n,j}| \leq c_2 n^{\alpha-1}, \quad j = 0, \dots, s$$

with some constants $c_1, c_2 > 0$. Furthermore, for sufficiently small h , there exists a constant C_1 such that

$$\left| (1 - h^\alpha \omega_0 K(x_n, x_n))^{-1} \right| \leq C_1 < \infty.$$

Since $K(t, x) \leq K_0 < \infty$ is assumed to be bounded on the interval in question, we get

$$\begin{aligned} |e_n| \leq C_1 & \left(h^\alpha c_2 K_0 \sum_{j=s+1}^{n-1} (n-j)^{\alpha-1} |e_j| \right. \\ & \left. + h^\alpha K_0 \left(c_1 \sum_{j=0}^s n^{\alpha-1} |e_j| \right) + |E_n^\alpha[\phi_n]| \right), \quad n = s, \dots, N. \end{aligned}$$

For $n \geq s+1$ we note that $n^{\alpha-1} < (n-j)^{\alpha-1}$ holds for $j = 1, \dots, s$, such that

$$(4.86) \quad |e_n| \leq h^\alpha C_0 \sum_{j=0}^{n-1} (n-j)^{\alpha-1} |e_j| + C_1 |E_n^\alpha[\phi_n]|, \quad n = s+1, \dots, N$$

with

$$C_0 = 2C_1 K_0 \max\{c_1, c_2\}.$$

Assuming that the error $E_n^\alpha[\phi_n]$ satisfies $O(h^{p-\varepsilon})$ for $n = 1, \dots, N$, Lemma 4.3.16 gives:

$$e_n = O(h^{p-\varepsilon}), \quad n = 1, \dots, N \quad \text{as } h \rightarrow 0,$$

where we used the uniform convergence of the Mittag-Leffler function.

The remaining task consists in proving that the errors $E_n^\alpha[\phi_n]$ satisfy $O(h^{p-\varepsilon})$ as $h \rightarrow 0$. Consider a function $\phi_{k,j}(x) = x^{k+j\alpha}$, where $k+j\alpha$ is not in the set A , defined in (4.78). This implies that $k+j\alpha > p-1$ and by Definition 4.3.2 of convergence of a fractional multistep method and in particular the remark (4.46) we can deduce for the convolution error ${}_h E^\alpha$ of $\phi_{k,j}$:

$${}_h E^\alpha \phi_{k,j}(x) = O(x_n^{k+(j+1)\alpha-p} h^p), \quad n = 1, \dots, N, \quad (x_n = nh)$$

Because of the construction of the starting weights it follows that

$$E_n^\alpha[\phi_{k,j}] = O(x_n^{k+(j+1)\alpha-p} h^p), \quad n = 1, \dots, N, \quad k+j\alpha \notin A.$$

Thus by

$$k + (j+1)\alpha - p = k + j\alpha + \alpha - p > p-1 + \alpha - p = \alpha - 1$$

we get

$$E_n^\alpha[\phi_{k,j}] = O(h^{p-\varepsilon}), \quad \text{with } 0 \leq \varepsilon < 1 - \alpha.$$

The structure (4.77) of the exact solution y finally leads to

$$E_n^\alpha[\phi_n] = O(h^{p-\varepsilon}), \quad \text{with } 0 \leq \varepsilon < 1 - \alpha, \quad n = 1, \dots, N.$$

With the above discussion we may write

$$(4.87) \quad \varepsilon = p - \alpha - \min\{\gamma = k + j\alpha, k, j \in \mathbb{N}_0, \gamma > p-1\}$$

and thus gain $\varepsilon \leq 0$ for the special case $\alpha = q/(q+1)$ with $q \in \mathbb{N}$. But by the order of the underlying classical multistep method the convergence error is bounded by $O(h^p)$ resulting in the lower bound $\varepsilon \geq 0$ finalizing the proof. \square

Remark 4.3.3 *a) The assumption of linearity of the kernel in proof of Theorem 4.3.15 is in fact only used for ease of notation. For the nonlinear case we may write $K_y(x_n, x_j, z_j)e_j$ instead of $K(x_n, x_j)e_j$ in equation (4.85), where, by the Mean-Value Theorem, z_j denotes an appropriate value between $y(x_j)$ and y_j .*

b) Equation (4.87) states that ε is dependent on the value of α as well as the order p of the underlying convolution quadrature. The worst cases (i.e. the largest value for ε) are obviously reached if $k + j\alpha$, $k, j \in \mathbb{N}_0$ is greater, but as close as possible to $p - 1$.

c) The results of Theorem 4.3.15 also hold for $\alpha \geq 1$, where the error behaves as $O(h^{p-\varepsilon})$ with $0 \leq \varepsilon \leq 1$.

Chapter 5

Numerical methods for fractional differential equations

Over the last decades the use of fractional order derivatives has become more and more attractive in the broad field of engineering to describe different kinds of models. We will look at some of these models in Chapter 6. The fractional operators and the corresponding differential and integral equations are usually chosen for the memory effect provided by their analytic properties described in the previous chapter. But if it comes to gaining a solution for a mathematical problem derived from a real life model, the theoretical results are usually not directly applicable for the given problems. Thus, as in the integer case, such problems are tackled with numerical methods, which themselves are based on the theoretical results of the previous chapters.

In Chapter 2.2 we have briefly discussed some numerical methods for the solution of integer order ordinary differential equations. In this chapter we will develop a number of numerical methods for fractional order ordinary and partial differential equations. These methods will be based on the ideas for the integer order case but due to the non-local character of fractional derivatives they will differ in important aspects and exhibit problems not known in the classical case.

Before starting the investigations, we need to give a note of caution. We have seen in the previous chapters that in general there exists more than one way to transfer results of classical calculus to the fractional case, which lead e.g. to the different definitions of fractional derivatives. This behaviour will become even more severe when we analyze numerical methods. It is common to construct methods for fractional differential equations by taking methods for classical (typically first-order) equations and then to generalize the concepts in an appropriate way. The obvious way to denote these methods is then to give them the same name as the underlying classical algorithm, possibly extended by the adjective “fractional”. As we will see, classical numerical schemes can be extended in more than one way, which may lead to the problem that, in two different items of literature, two different algorithms are denoted by the same name. Of course, this is a potential source for confusion, and the reader must be very careful in this respect.

This problem becomes even more complicated by the fact that fractional derivatives

have non-local character. Thus, given for example, the equation

$$D_*^\alpha y(x) = f(x, y(x))$$

combined with some appropriate initial conditions, we may use Lemma 4.2.3 2. to rewrite the initial value problem in the form of a Volterra integral equation. Then we may try to solve this Volterra equation by some (properly generalized) algorithm for Volterra problems and give the name of this fundamental algorithm to the entire scheme. On the other hand it is also possible to recall the definition of the Caputo differential operator D_*^α (concatenation of integral operator and differential operator). In this way we see that the equation itself is a Volterra integro-differential equation, and we may handle it as such. Finally it is possible (cf. Lemma 5.1.2) to express the operator D_*^α in a different way, namely as a (strongly singular) Volterra integral operator. Then, the equation already is a Volterra equation and may be solved numerically by an appropriately modified algorithm for Volterra equations. So, given an algorithm for the numerical solution of Volterra equations, we have at least three different options for the generalization of this algorithm to our fractional differential equation, and it is not unlikely that in the literature these three different methods will be given the same name, viz. the name of the underlying Volterra equation algorithm.

We will try to circumvent these naming problems by denoting the methods on the one hand by the underlying classical method, and on the other hand adding the name of the author, who should be given credits for introducing the method. Of course, the last aspect is a problem by itself, since more than once the origin of a fractional numerical method can be traced back to various authors; we will use the name of the authors we think most influential on the development of the method in question.

Bearing in mind these warnings, we now outline the structure of the following chapters where these matters will be discussed. We begin in Chapter 5.1 with a repetition of the type of problems we are interested to solve numerically. We will then describe in detail three different methods for a fractional formulation of backward difference methods. We start in Chapter 5.1.1 with a direct approach to fractional order backward differences which is based on the structure of the finite Grünwald-Letnikov operator introduced in Theorem 4.1.30. In the following Chapter 5.1.2 we will present a slightly different approach based on a direct discretization of the given fractional differential equation. To be more precise we will show in which way the Caputo differential operator can be understood directly as an integral, to which we apply quadrature techniques in order to construct the backward difference method. We will close the analytical examination of backward difference techniques in Chapter 5.1.3 with the general class of high-order backward difference methods based on the analytical results of fractional linear multistep methods stated in Chapter 4.3. A different numerical approach will be given in Chapter 5.2, where we will introduce a method, which computes the asymptotic expansion of the solution of a fractional order differential equation. On the one hand this will be a numerical method by itself (by only computing the first terms of the expansion) but more importantly it will give us a way to circumvent problems in practical computation of higher-order methods as described in Chapter 5.1.3. The whole problem complex of implementation of higher-order methods will be addressed in Chapter 5.3.

A last numerical method also based on a fractional linear multistep method will be addressed in Chapter 5.4, where we will introduce a fractional Adams method (see e.g. Example 2.2.1 for the classical case).

We will close our analysis of numerical methods with a chapter on possible improvements of the stated numerical algorithms.

5.1 Fractional backward difference methods

In this section we want to develop numerical algorithms for the solution of the fractional order differential equation of Riemann-Liouville type

$$(5.1) \quad D^\alpha y(x) = f(x, y(x)), \quad D^{\alpha-k} y(0) = b_k \quad k = 1, 2, \dots, n-1, \quad \lim_{z \rightarrow 0+} J^{n-\alpha} y(z) = b_n$$

and more importantly (for their practical use) Caputo type

$$(5.2) \quad D_*^\alpha y(x) = f(x, y(x)), \quad D^k y(0) = b_k \quad (k = 0, 1, \dots, n-1),$$

where $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. We are interested in a solution $y(x)$ for equation (5.1) or (5.2) on a closed interval $[0, X]$ for some $X > 0$. As in the classical case the numerical methods are not supposed to produce a solution on the whole interval in question, but rather give the solution on a prescribed set of nodes on the given interval. We assume that the nodes are arranged equispaced inside the interval $[0, X]$ and on its borders with a given stepsize h . Additionally the nodes are assumed to be numbered increasingly x_0, x_1, \dots, x_N , where $N = X/h$, $x_0 = 0$ and $x_N = X$. Furthermore we denote by y_m the approximation of $y(x_m)$ and equally $f_m = f(x_m, y_m)$ as the discretized right-hand side of the differential equation in question. For this setting we will develop the fractional counterpart of the well known classical backward difference method. We will see that, as for the fractional operators themselves, there exists more than one way to carry over the classical ideas to the fractional setting. We begin with the most obvious one, based on the Grünwald-Letnikov derivative.

5.1.1 Backward differences and the Grünwald-Letnikov definition

Instead of considering either problem (5.1) or (5.2) directly let us start with a formally different third one given by

$$(5.3) \quad {}^{GL}D^\alpha y(x) = f(x, y(x)), \quad y(0) = 0, \quad 0 < \alpha < 1,$$

where the Grünwald-Letnikov differential operator is used. Since we prescribed a homogeneous initial condition we know by Corollary 4.1.29 that problem (5.3) is equivalent to problems (5.1) and (5.2) for the given case $0 < \alpha < 1$. The advantage of the problem formulation (5.3) is, that we gain an immediate discretization technique from the definition of the Grünwald-Letnikov derivative

$${}^{GL}D^\alpha y(x) = \lim_{h \rightarrow 0} \frac{(\Delta_h^\alpha y)(x)}{h^\alpha} = \lim_{\substack{h \rightarrow 0 \\ \ell h = x}} \frac{1}{h^\alpha} \sum_{k=0}^{\ell} (-1)^k \binom{\alpha}{k} y(x - kh), \quad \alpha > 0.$$

If we do not perform the limit operation $h \rightarrow 0$, we get the *finite* Grünwald-Letnikov operator

$${}_F^{GL}D^\alpha y(x_m) = \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} y(x_m - kh), \quad m = 0, 1, \dots, N,$$

which thus gives us a discretized version of the operator ${}^{\text{GL}}D^\alpha$. Using the defined mesh points x_0, \dots, x_N we therefore get the discretized problem

$$\frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} y(x_m - kh) = f(x_m, y(x_m)), \quad m = 0, 1, \dots, N.$$

If we set $\omega_k = (-1)^k \binom{\alpha}{k}$ we can solve this set of equations one by one at each mesh point x_m by

$$(5.4) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh), \quad m = 1, \dots, N.$$

This formula computes the numerical solution of the fractional order differential equation (5.3): Obviously the solution we seek at each step, namely y_m , occurs on both sides of equation (5.4). But in each step the m th equation contains y_m as the only unknown quantity, because we have computed y_1, y_2, \dots, y_{m-1} in the previous calculations and the solution $y_0 = 0$ is determined by the initial condition in (5.3). Therefore we can solve formula (5.4) for all $m = 1, \dots, N$ in a step by step manner. Of course, in the general case the equations will still be nonlinear, and so we will have to use a (one-dimensional) fixed point method to solve each of them individually.

From Theorem 4.1.30 we know that for the problem (5.3) the finite Grünwald-Letnikov operator gives a first order approximation to the Riemann-Liouville differential operator and by the choice of the homogenous initial condition in (5.3) also to the Caputo differential operator. Thus formula (5.4) gives us a first order numerical method to solve equations of the type (5.3) as well as equations of type (5.1) and (5.2) given that $0 < \alpha < 1$ and the initial condition is homogenous.

Before we generalize problem (5.3) to the case, where $\alpha > 0$ and the corresponding initial conditions are not necessary homogenous, we take a closer look at the weights ω_k of the finite Grünwald-Letnikov derivative.

The coefficients ω_k can be computed in a recursive scheme (with $\omega_0 = 1$) by

$$(5.5) \quad \begin{aligned} \omega_k &= (-1)^k \binom{\alpha}{k} = (-1)^k \frac{\Gamma(\alpha + 1)}{\Gamma(k + 1)\Gamma(\alpha - k + 1)} \\ &= -(-1)^{k-1} \frac{\Gamma(\alpha + 1)(\alpha - k + 1)}{k\Gamma(k)\Gamma(\alpha - k)} = \left(\frac{k - (\alpha + 1)}{k} \right) \omega_{k-1} \\ &= \left(1 - \frac{\alpha + 1}{k} \right) \omega_{k-1} \end{aligned}$$

for all $k \in \mathbb{N}$. Another way to compute the coefficients ω_k is by their generating function

$$(5.6) \quad \omega(\zeta) = (1 - \zeta)^\alpha,$$

i.e. the first k Taylor coefficients of (5.6) are the first k weights ω_k , which lead by automatic differentiation techniques (see Theorem 5.3.1) to the same recursive formula (5.5). Thus on first sight we do not gain new information from the generating function. But on a second look we ascertain that the generating function (5.6) is the generating function of the first order backward difference method (see formula (2.12)) for the case $\alpha = 1$. Thus we know by

Theorem 4.3.11 that formula (5.4) is convergent of order 1 in the sense of Definition 4.3.2. This fact seems to be widely misunderstood to imply that the *error* of formula (5.4) should behave as $O(h)$ for a finite h . This interpretation is of course not entirely correct as we see by investigating Corollary 4.3.14, which states that we need one additional starting weight at each step (see also Chapter 5.1.3) given by

$$(5.7) \quad \begin{aligned} w_m &= \frac{m^{-\alpha}}{\Gamma(1-\alpha)} - (-1)^m \frac{\Gamma(\alpha)}{\Gamma(\alpha-m)\Gamma(m+1)} \\ &= \frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^m \omega_j, \end{aligned}$$

resulting in a slightly modified formula

$$(5.8) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh) - \left(\frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^m \omega_j \right) y_0, \quad m = 1, \dots, N,$$

whose error behaves like $O(h)$. Obviously formulas (5.4) and (5.8) are identical if homogenous initial conditions are given, which might be the reason behind the mentioned misunderstanding.

We now expand the class of problems we are going to solve with this first backward difference scheme and consider problem (5.3) with $\alpha > 0$ and the corresponding (not necessarily homogenous) initial conditions given either in Riemann-Liouville or Caputo form. These kinds of problems are in part smartly solved in a recent paper by Podlubny [123], where he used a so called matrix approach. We therefore take a moment to give a brief outline of his method and point out some minor errors and more importantly its restriction to *linear* problems.

Excursus 2 (Podlubny's matrix approach) *The basic idea of Podlubny's matrix approach in [123] is based on the fact that given a fractional differential equation with homogenous initial conditions we can write formula (5.4) for all nodes y_m simultaneously in a matrix representation as*

$$(5.9) \quad \frac{1}{h^\alpha} \begin{pmatrix} \omega_0 & & & \\ \omega_1 & \omega_0 & & \\ \vdots & \vdots & \ddots & \\ \omega_N & \omega_{N-1} & \dots & \omega_0 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_N \end{pmatrix} \Leftrightarrow B_N^\alpha Y_N = F_N.$$

Since $y_0 = 0$ is known from the initial condition, we discard the first equation of this equation system (i.e. the first row of B_N^α and the first entry in F_N) and then solve the fractional differential equation at each node simultaneously by solving the remaining equation system instead of using the apparent unwieldy recurrence formula (5.4), which solves at each node step by step.

While this method is a plausible and elegant approach to the given problem, one has to be careful in which way it is restricted (and it is stated even slightly erroneous in parts in [123]): Podlubny described his method for linear k -term fractional differential equations (i.e. equations containing more than one fractional differential operator) with homogenous or

inhomogeneous initial conditions of either Riemann-Liouville or Caputo type. The fact that he describes his method for k -term equations broadens the types of problems one can solve and the basic idea of discretizing all occurring differential operators in a k -term problem by the described formula (5.4) is straight forward and does not complicate the method. The restriction to linear problems on the other hand is both necessary and limiting for the method.

The necessity to consider only linear problems is founded by the fact that for such problems any inhomogeneous initial conditions can be transferred to homogenous ones by replacing $y(x)$ with

$$(5.10) \quad y(x) = \sum_{k=0}^{n-1} b_k x^k + z(x) \quad \text{or} \quad y(x) = \sum_{k=1}^n b_k x^{\alpha-k} + z(x)$$

for the case of Caputo and Riemann-Liouville initial conditions respectively, and then solve the problem for the new unknown function $z(x)$. This transformation obviously leads to a fractional order differential equation with homogenous initial conditions which can be solved by the equation system (5.9). But the described transformation is in general only possible if the right-hand side of the given problem is linear so the restriction to linear problems is in fact a necessity in Podlubny's approach, while inhomogeneous initial conditions do not pose a problem since they can be transformed to homogenous ones.

The described method works for any linear problem with $\alpha > 0$, but it seems like only one of the given $n = \lceil \alpha \rceil$ initial conditions in the whole method has been used. Podlubny wrongly states that the remaining homogenous initial conditions give the solution at the corresponding number of first nodes, which supposedly are all zero. In truth we already have used the remaining initial conditions which will become evident when we now look at the backward difference method for general problems.

From now on we will mainly focus on general problems of Caputo type, i.e. we are interested in a numerical solution to the problem (5.2). The Riemann-Liouville type of fractional differential equations is less common in applications due to the fact that the necessary initial conditions are not of classical type, i.e. information about the fractional derivative at the starting point x_0 is needed, which often has no known physical meaning and/or cannot be measured, as opposed to the classical integer order initial conditions in the Caputo case. However some of the upcoming numerical methods can be transferred to the Riemann-Liouville type and we will address these transformations in remarks.

From Corollary 4.1.29 we know that in general the Grünwald-Letnikov operator and the Caputo operator are connected by

$$\begin{aligned} D_*^\alpha y(x) &= {}^{GL}D^\alpha (y(x) - T_{n-1}[y; 0](x)) \\ &= {}^{GL}D^\alpha y(x) - D^\alpha T_{n-1}[y; 0](x) \end{aligned}$$

where $y(x)$ is assumed to be n times continuously differentiable. Applied to our problem (5.2) the Taylor polynomial $T_{n-1}[y; 0](x)$ is completely defined by the initial conditions and thus we can rewrite formula (5.8) in the case of $\alpha > 0$ to

$$(5.11) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh) - \left(\frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^m \omega_j \right) y_0$$

$$+h^\alpha D^\alpha T_{n-1}[y;0](x_m), \quad m = 1, \dots, N.$$

All the arguments we stated on formulas (5.4) and (5.8) still apply. We thus have obtained a numerical method of first order to solve fractional differential equations of Caputo type with linear or nonlinear right-hand side and homogenous or inhomogeneous initial conditions for all $\alpha > 0$.

Remark 5.1.1 *a) We note that the derivative $D^\alpha T_{n-1}[y;0](x)$ in formula (5.11) can be calculated by Example 4.1.2:*

$$D^\alpha T_{n-1}[y;0](x_m) = \sum_{k=0}^{n-1} \frac{b_k x_m^{k-\alpha}}{\Gamma(k+1-\alpha)}.$$

b) From studying formula (5.11) for the nonlinear Caputo cases it is obvious, where the initial conditions $y^{(k)}(0) = y_k$, $k = 1, \dots, n-1$ have been used in the linear case of Podlubny's matrix approach: The Taylor polynomial in formula (5.11) equals zero in case of homogenous initial conditions and therefore the equation system (5.9) stays the same for $\alpha > 1$ as for $0 < \alpha \leq 1$.

b) Considering equations of Riemann-Liouville type (5.1) results in a formula similar to (5.11). Again we know the connection between the two operators, i.e. Riemann-Liouville and Grünwald-Letnikov, from Corollary 4.1.29. It states that they are identical but we might use a slightly more complex identity, given as

$$D^\alpha y(x) = D^\alpha (y(x) - \hat{T}_{n-1}[y;0](x)),$$

where

$$(5.12) \quad \hat{T}_{n-1}[y;0](x) = \sum_{k=1}^n \frac{b_k x^{\alpha-k}}{\Gamma(\alpha-k+1)}$$

is the Riemann-Liouville analog to the Taylor expansion in the Caputo case, and b_k , $k = 1, \dots, n$ are the Riemann-Liouville initial conditions. The function $\hat{T}_{n-1}[y;0](x)$ obviously lies in the kernel of D^α , so that we have in fact only written down a more complex identity. Thus we get formula (5.11) for the Riemann-Liouville case, where T is replaced by \hat{T} . But the structure of the Riemann-Liouville initial conditions does not allow us in general to start with the solution $y(0) = b_0$, since this value is not given in the initial conditions and might not even exist (see Remark 4.2.1). Thus the above method works fine for fractional order differential equations of Caputo type but does not work directly for Riemann-Liouville operators unless the initial conditions are homogenous.

Summarizing our numerical methods based on fractional backward differences so far we can ascertain:

First order numerical methods (Error behaves as $O(h)$ at each mesh point $x_m, m = 1, 2, \dots, N$):

- A (non)linear fractional order differential equation of either Riemann-Liouville or Caputo type with $\alpha > 0$ and homogenous condition(s) can be solved by formula (5.4), where in each step $m = 1, \dots, N$ a (non)linear equation has to be solved.
- A linear fractional order differential equation of either Riemann-Liouville or Caputo type with $\alpha > 0$ and inhomogeneous initial condition(s) can be transferred to a corresponding equation with homogenous conditions by the transformation given in (5.10) and then be solved by formula (5.4) where in each step $m = 1, \dots, N$ a linear equation has to be solved.
- A nonlinear fractional order differential equation of Caputo type with $\alpha > 0$ and inhomogeneous initial condition(s) can be solved by formula (5.8).
- For a nonlinear fractional order differential equation of Riemann-Liouville type with $\alpha > 0$ and inhomogeneous initial condition(s) none of the above formulas can be applied directly.

We have established a first fractional backward difference method, which we can use to solve fractional order differential equations. We will derive a different approach transferring the idea of backward differences to the fractional case in the next chapter. But we will come back to the method described here in Chapter 5.1.3.

5.1.2 Diethelm's fractional backward differences based on quadrature

The numerical method we are going to describe in this chapter can be considered as a second way to construct a fractional backward difference method. For linear equations this method was independently introduced by Chern [24] and Diethelm [31]. The latter paper also contains detailed error analysis for the linear case, which is the reason for denoting this method as *Diethelm's fractional backward difference method*. The following description of this method will be taken in parts directly from [33, Ch. 7], where the results of [31] are presented under more general assumptions.

Before we begin our main investigation we need to state rather uncommon representations of the Riemann-Liouville and Caputo derivatives:

Lemma 5.1.1 *Let $\alpha > 0$, $\alpha \notin \mathbb{N}$, and $n = \lceil \alpha \rceil$. Assume that $f \in C^n[0, X]$ and $x \in [0, X]$. Then,*

$$(5.13) \quad D^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \int_0^x (x-t)^{-\alpha-1} f(t) dt.$$

In this statement, the integral needs some further explanation. The integrand exhibits a singularity of order $1 + \alpha$ which is strictly greater than one, and thus the integral will

in general exist neither in the proper nor in the improper sense. Therefore, we define such an integral according to Hadamard's finite-part integral concept as explained e.g. in the Appendix C of [33]. For a proof of this lemma we also refer to [33, Lem. 2.18]. An immediate consequence is given by

Lemma 5.1.2 *Under the assumptions of Lemma 5.1.1, we have*

$$(5.14) \quad D_*^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \int_0^x (x-t)^{-\alpha-1} (f(t) - T_{n-1}[f;0](t)) dt.$$

The representation (5.14) for the Caputo derivative is simpler than its basic definition (4.7) since instead of two operators (a differential and an integral operator) only a single integral operator is used. Even though this integral is defined only by means of special regularization, it still is essentially an integral and therefore we can use quadrature theory known from classical calculus in a quite direct way.

The following results have first been presented in [32]: Applying the linear transformation $t = xu$ to (5.13) we find that

$$(5.15) \quad D^\alpha f(x) = \frac{x^{-\alpha}}{\Gamma(-\alpha)} \int_0^1 u^{-\alpha-1} g(u) du, \quad \text{for all } x \in (0, X],$$

where $g(u) = f(x - xu)$. Therefore, we can shift our attention to the approximation of the finite-part integral

$$(5.16) \quad \int_0^1 u^{-\alpha-1} g(u) du$$

whose singularity is located at the origin.

For the numerical approximation of the integrals of the form (5.16), we want to use *compound quadrature formulas* of degree $d \in \mathbb{N}_0$, i.e. we proceed in the following way: First, we define a mesh $0 = x_0 < x_1 < \dots < x_j = 1$. Then, we construct a function \tilde{g}_d that interpolates our function g as follows. On every subinterval $[x_{\nu-1}, x_\nu]$ ($\nu = 1, 2, \dots, j$), the function \tilde{g}_d is defined to be the d th degree polynomial that interpolates g in the (equidistant) nodes $x_{\nu-1} + \mu(x_\nu - x_{\nu-1})/d$, $\mu = 0, 1, \dots, d$. For $d = 0$, we only use the node $x_{\nu-1}$. The piecewise polynomial \tilde{g}_d is then integrated exactly in the finite-part sense with respect to the weight function $u^{-\alpha-1}$. Thus, we obtain our desired approximation

$$Q_j[g] := \int_0^1 u^{-\alpha-1} \tilde{g}_d(u) du.$$

We remark that, following our construction, it is clear that $Q_j[g]$ depends not only on j but also on the degree d of the piecewise polynomials, on the order α of the differential operator, and on the choice of the mesh points x_0, x_1, \dots, x_j .

The formula Q_j has got $dj + 1$ nodes if $d \geq 1$, and j nodes for $d = 0$. Since, in practical applications, the value d will usually be fixed and j may increase, it is obvious that j is a measure for the computational effort required for the evaluation of $Q_j[g]$.

In theory there may be certain advantages in choosing the mesh points x_1, x_2, \dots, x_{j-1} in a specific non-equispaced way (cf. [32, §3]) when one is only looking for an approximation for the fractional derivative. In practice however, there are major disadvantages to this

approach from the numerical point of view as explained in [32, §4]; moreover, when it comes to the application of our scheme to the solution of fractional differential equations, it is also much more convenient to use a uniform mesh. Therefore, we shall concentrate on the latter and assume for the moment that

$$x_k = k/j, \quad k = 0, 1, \dots, j.$$

We now want to analyze the error introduced by this approximation scheme. In order to do this, we need to impose certain smoothness assumptions on the integrand function g . As usual in approximation theory, we will assume that $g \in C^n[0, 1]$ for some $n \in \mathbb{N}^1$. We may note here that the smoothness properties of f in (5.13) and g in (5.15) are directly connected and in particular $g \in C^n[0, 1]$ if $f \in C^n[0, X]$. The analysis will show that the error will depend on the precise values of the order α of the differential operator, on the smoothness order n of the function g , and on the order d of the piecewise polynomials that we shall use. In particular, for reasons explained in more detail in [32, §1], it is only possible to find bounds of the form we are interested in under the assumption that

$$(5.17) \quad \alpha < n \leq d + 1.$$

Henceforth we will assume these inequalities to be satisfied.

The case $d = 1$ (piecewise linear interpolation) will be the most important to us, so we shall discuss it in a more detailed way. The other cases will be covered rather briefly. For this special case, we have the following result:

Theorem 5.1.3 *Let $n \in \{1, 2\}$, $d = 1$, and $\alpha \in (0, 2) \setminus \{1\}$ such that (5.17) is satisfied. Then, there exists a constant $\gamma_{\alpha, n, j}$ depending only on α , n , and j , such that for all $g \in C^n[0, 1]$ we have*

$$\left| \int_0^1 u^{-\alpha-1} g(u) du - Q_j[g] \right| \leq \gamma_{\alpha, n, j} \|g^{(n)}\|_\infty$$

and

$$\gamma_{\alpha, n, j} = O(j^{\alpha-n}).$$

The proof for this result can be found in [33, Thm. 7.1] and the proof for the following more general result is given in [33, Thm. 7.2]:

Theorem 5.1.4 *Assume $0 < \alpha \notin \mathbb{N}$ and let $n \in \mathbb{N}$ and $d \in \mathbb{N}_0$ be such that (5.17) is satisfied. Then, there exists a constant $\gamma_{\alpha, n, j, d}$ depending only on α , n , j , and d , such that for all $g \in C^n[0, 1]$ we have*

$$\left| \int_0^1 u^{-\alpha-1} g(u) du - Q_j[g] \right| \leq \gamma_{\alpha, n, j, d} \|g^{(n)}\|_\infty$$

and

$$\gamma_{\alpha, n, j, d} = O(j^{\alpha-n}).$$

¹As from now we use in this section the variable n as an arbitrary natural number, which is not necessarily equal to $\lceil \alpha \rceil$. Since we will only need the term $\lceil \alpha \rceil$ to describe the Taylor polynomial $T_{\lceil \alpha \rceil - 1}$ in this section, we refrain to introduce another variable to describe the differentiability properties of the functions f and g .

Combining the results obtained in this chapter, we have so far found an approximation for the Caputo fractional derivative in the following way,

$$D_*^\alpha y(x) \approx \frac{x^{-\alpha}}{\Gamma(-\alpha)} Q_j[g],$$

where

$$g(u) = y(x - xu) - T_{[\alpha]-1}[y; 0](x - xu)$$

with $x > 0$, and we have analyzed the corresponding error term. This is what we now want to use as a building block for an algorithm for the numerical solution of fractional differential equations. For this purpose it is useful to give a more explicit representation for Q_j . Specifically we want to pursue this idea in detail for the case $d = 1$.

Lemma 5.1.5 *For $d = 1$ (piecewise linear interpolation), we have*

$$Q_j[g] = \sum_{k=0}^j \omega_{kj} g(k/j)$$

with

$$\alpha(1-\alpha)j^{-\alpha}\omega_{kj} = \begin{cases} -1 & \text{for } k = 0, \\ \alpha & \text{for } k = j = 1, \\ 2 - 2^{1-\alpha} & \text{for } k = 1 \text{ and } j \geq 2, \\ 2k^{1-\alpha} - (k-1)^{1-\alpha} - (k+1)^{1-\alpha} & \text{for } 2 \leq k \leq j-1, \\ (\alpha-1)k^{-\alpha} - (k-1)^{1-\alpha} + k^{1-\alpha} & \text{for } k = j \geq 2. \end{cases}$$

Proof: It is clear by construction that Q_j can be represented as a weighted sum of function values of the integrand, taken at the points k/j .

For $k \in \{0, 1, \dots, j\}$ we introduce the fundamental functions

$$\phi_{kj}(x) := \begin{cases} jx - (k-1) & \text{for } x \in [(k-1)/j, k/j], \\ k+1 - jx & \text{for } x \in (k/j, (k+1)/j], \\ 0 & \text{else.} \end{cases}$$

The main properties of these functions are easily seen to be

- $\phi_{kj} \in C[0, 1] \cap C^\infty[0, 1/j]$,
- $\phi_{kj}(v/j) = 0$ for $v \in \{0, 1, 2, \dots, j\} \setminus \{k\}$,
- $\phi_{kj}(k/j) = 1$.

The first of these properties asserts that the integrals $\int_0^1 u^{-\alpha-1} \phi_{kj}(u) du$ exist for all k . Moreover, by construction of the quadrature formula Q_j ,

$$\int_0^1 u^{-\alpha-1} \phi_{kj} du = Q_j[\phi_{kj}] = \sum_{v=0}^j \omega_{vj} \phi_{kj}(v/j) = \omega_{kj}$$

in view of the second and third property of ϕ_{kj} . Taking into consideration that ϕ_{kj} is zero over $j-2$ subintervals of $[0, 1]$ and a first-degree polynomial over each of the other two subintervals, it is easy to calculate the integrals $\int_0^1 u^{-\alpha-1} \phi_{kj}(u) du$ explicitly and thus to come up with the required expressions for the ω_{kj} . \square

Given this information, we now present the remaining parts of the derivation of Diethelm's backward difference method for the fractional differential equation of Caputo type (5.2). In view of the fact that, at present, we only discuss the scheme for $d = 1$ (quadrature based on piecewise linear interpolation), relation (5.17) forces us to restrict the order α of the differential equation to be in the range $0 < \alpha < 2$. This means that, in order to obtain a unique solution, we need to specify initial conditions

$$(5.18) \quad \begin{cases} y(0) = b_0 & \text{if } 0 < \alpha < 1, \\ y(0) = b_0, \quad y'(0) = b_1 & \text{if } 1 < \alpha < 2. \end{cases}$$

Finally, we assume that the given function f on the right-hand side of (5.2) fulfills the hypotheses of Theorem 4.2.2; specifically this means continuity and a Lipschitz condition with respect to the second variable. Then we can be sure that a unique solution exists over some interval $[0, X]$.

The algorithm now proceeds as follows: Choose a positive integer N and divide the interval $[0, X]$ into N subintervals of equal length $h = X/N$ with breakpoints $x_m := mh$, $m = 0, 1, \dots, N$. Next, we write up the equation (5.2) for $x = x_m$, $m = 1, 2, \dots, N$, using the identity (5.15). This yields

$$\begin{aligned} f(x_m, y(x_m)) &= D_*^\alpha y(x_m) = D^\alpha y(x_m) - D^\alpha T_{[\alpha]-1}[y; 0](x_m) \\ &= \frac{x_m^{-\alpha}}{\Gamma(-\alpha)} \int_0^1 u^{-\alpha-1} y(x_m - x_m u) du - D^\alpha T_{[\alpha]-1}[y; 0](x) \\ &= \frac{x_m^{-\alpha}}{\Gamma(-\alpha)} \int_0^1 u^{-\alpha-1} y(x_m - x_m u) du - \frac{b_0 x_m^{-\alpha}}{\Gamma(1-\alpha)} - \frac{b_1 x_m^{1-\alpha}}{\Gamma(2-\alpha)}, \end{aligned}$$

where we have also taken into account the definition of the Caputo derivative and the fact that we can calculate the Riemann-Liouville derivative of the Taylor polynomial $T_{[\alpha]-1}[y; 0]$ explicitly (the Taylor polynomial is known in view of the given initial values). Here and in the following we tacitly set $b_1 := 0$ in the case $0 < \alpha < 1$; this allows us to treat both cases ($\alpha < 1$ and $\alpha > 1$) simultaneously. In this relation we replace the integral by the quadrature formula Q_m , additionally introducing the quadrature error R_m . Thus, using the abbreviation $g_m(u) := y(x_m - x_m u)$, this yields

$$(5.19) \quad \frac{x_m^{-\alpha}}{\Gamma(-\alpha)} \left(\sum_{k=0}^m \omega_{km} g_m(k/m) + R_m[g_m] \right) - \frac{b_0 x_m^{-\alpha}}{\Gamma(1-\alpha)} - \frac{b_1 x_m^{1-\alpha}}{\Gamma(2-\alpha)} = f(x_m, y(x_m)).$$

Now we need to consider some approximations for the unknown quantities in this equation. First, note that

$$g_m(k/m) = y((m-k)h),$$

where the exact solution $y((m-k)h)$ is not known except for the special case $m = k$ that corresponds to the given initial value. The quadrature error is not known either. Finally, since $y(x_m)$ is presently unknown, we cannot evaluate the right-hand side of (5.19). Therefore, we assume that we have approximations y_ν for the values $y(x_\nu)$ at least for $\nu = 0, 1, \dots, m-1$, and introduce these into (5.19). Moreover, we simply ignore the quadrature error. The remaining unknown quantity is then $y(x_m)$, and since we have perturbed the equation, the

solution of this new equation y_m , say, will only be an approximation for $y(x_m)$. This value is defined (implicitly) by being the solution of the equation

$$(5.20) \quad \frac{x_m^{-\alpha}}{\Gamma(-\alpha)} \sum_{k=0}^m \omega_{km} y(x_m - kh) - \frac{b_0 x_m^{-\alpha}}{\Gamma(1-\alpha)} - \frac{b_1 x_m^{1-\alpha}}{\Gamma(2-\alpha)} = f(x_m, y_m).$$

Now we need to justify our assumption that the required approximations y_v are known: First we calculate y_1 by means of (5.20). To do this we only need to have an approximation y_0 for $y(x_0)$; this is given by the initial condition. To calculate y_2 we need to know y_1 and y_0 ; those two values have just been found. Obviously, we can proceed in this iterative manner, so all the necessary ingredients are available.

In order to investigate the properties of this method further, it will be helpful to rewrite equation (5.20) in the following way:

$$\begin{aligned} & \frac{x_m^{-\alpha}}{\Gamma(-\alpha)} \sum_{k=0}^m \omega_{km} y(x_m - kh) - \frac{b_0 x_m^{-\alpha}}{\Gamma(1-\alpha)} - \frac{b_1 x_m^{1-\alpha}}{\Gamma(2-\alpha)} = f(x_m, y_m) \\ \Leftrightarrow & \frac{(mh)^{-\alpha}}{\Gamma(-\alpha)} \sum_{k=0}^m \omega_{km} y(x_m - kh) - \frac{b_0 (mh)^{-\alpha}}{\Gamma(1-\alpha)} - \frac{b_1 (mh)(mh)^{-\alpha}}{\Gamma(2-\alpha)} = f(x_m, y_m) \\ \Leftrightarrow & \sum_{k=0}^m \omega_{km} y(x_m - kh) = \Gamma(-\alpha)(mh)^\alpha f(x_m, y_m) + \frac{\Gamma(-\alpha)}{\Gamma(1-\alpha)} b_0 + \frac{mh\Gamma(-\alpha)}{\Gamma(2-\alpha)} b_1. \end{aligned}$$

Substituting

$$(5.21) \quad \omega_{km} = \frac{\tilde{\omega}_{km} \Gamma(2-\alpha)}{-\alpha(1-\alpha)m^{-\alpha}}$$

yields

$$\begin{aligned} \sum_{k=0}^m \tilde{\omega}_{km} y(x_m - kh) &= h^\alpha f(x_m, y_m) + \frac{m^{-\alpha}}{\Gamma(1-\alpha)} b_0 + h \frac{m^{1-\alpha}}{\Gamma(2-\alpha)} b_1 \\ &= h^\alpha f(x_m, y_m) + h^\alpha \frac{x_m^{-\alpha}}{\Gamma(1-\alpha)} b_0 + h^\alpha \frac{x_m^{1-\alpha}}{\Gamma(2-\alpha)} b_1. \end{aligned}$$

We finally solve the left-hand side for y_m and get

$$(5.22) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \tilde{\omega}_{km} y(x_m - kh) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$$

where the weights $\tilde{\omega}_{km}$ are given by Lemma 5.1.5 and the substitution (5.21), i.e.

$$(5.23) \quad \frac{\tilde{\omega}_{km}}{\Gamma(2-\alpha)} = \begin{cases} 1 & \text{for } k = 0, \\ -\alpha & \text{for } k = m = 1, \\ 2^{1-\alpha} - 2 & \text{for } k = 1 \text{ and } m \geq 2, \\ (k-1)^{1-\alpha} + (k+1)^{1-\alpha} - 2k^{1-\alpha} & \text{for } 2 \leq k \leq m-1, \\ (k-1)^{1-\alpha} - (\alpha-1)k^{-\alpha} - k^{1-\alpha} & \text{for } k = m \geq 1. \end{cases}$$

If we formally set $\alpha = 1$ (which implies that we have to choose $b_1 = 0$) we get immediately

$$\tilde{\omega}_{0m} = 1, \quad \tilde{\omega}_{1m} = -1 \quad \text{and} \quad \tilde{\omega}_{km} = 0 \quad \text{for} \quad k \geq 2,$$

i.e. we recover the classical two-point backward differentiation formula for first-order equations, so that the described method can in fact be considered as a second generalization of the idea of backward difference formulas for the fractional case.

That Diethelm's fractional backward difference method is indeed different from the Grünwald-Letnikov approach can be seen by a simple comparison of formulas (5.11) and (5.22): We can rewrite formula (5.11) to match exactly the form of formula (5.22) by

$$(5.24) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \hat{\omega}_{km} y(x_m - kh) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$$

where the weights $\hat{\omega}_{km}$ are now given by

$$(5.25) \quad \hat{\omega}_{km} = \begin{cases} (-1)^k \frac{\Gamma(\alpha)}{\Gamma(k)\Gamma(\alpha - k + 1)} + \frac{k^{-\alpha}}{1 - \alpha} & \text{for } k = m \geq 0, \\ (-1)^k \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha + 1)\Gamma(\alpha + 1 - k)} & \text{for } 0 \leq k \leq m - 1. \end{cases}$$

Obviously the two sets of weights ($\tilde{\omega}_{km}$ and $\hat{\omega}_{km}$) are different, while the rest of formulas (5.22) and (5.24) are identical. But in the classical case of $\alpha = 1$ both retain the structure of the first order backward differentiation formula.

Remark 5.1.2 *The easiest way to check if the two sets of weights $\tilde{\omega}_{km}$ and $\hat{\omega}_{km}$ are different is by choosing a rational value for α . Then apart from the case $k = m \geq 0$ all weights $\hat{\omega}_{km}$ are also rational, while they are non-rational numbers for $\tilde{\omega}_{km}$.*

Two important open questions remain with respect to formula (5.22): The first one is concerned with the solvability of equation (5.22) and the second one with the behaviour of the error for formula (5.22). Both questions are answered in [33, Ch. 7.2] for a special type of right-hand side, given by

$$f(x, y) = -\mu y + q(x)$$

with some $\mu > 0$ and some continuous function q . In addition to this restriction the following theorems are only proven in [33] for the case $0 < \alpha < 1$ but strong indications are made that they hold for the case $1 < \alpha < 2$ as well. We are not going to expand the results in [33] here, since our main numerical algorithms will be based on the Grünwald-Letnikov approach and its higher order variants, which will be described in the next chapter. However, for the sake of completeness and more importantly their use for numerical methods on partial differential equations of fractional order, we state them here:

Theorem 5.1.6 *Let $0 < \alpha < 1$ or $1 < \alpha < 2$. Assuming that $f(x, y) = -\mu y + q(x)$ with some continuous function q and some $\mu > 0$, equation (5.22) has a unique solution for every $h > 0$ (the length of the subintervals of the partition).*

Theorem 5.1.7 *Let $0 < \alpha < 1$. Assuming that $f(x, y) = -\mu y + q(x)$ with some continuous function q and some $\mu > 0$ being such that the solution $y \in C^2[0, T]$, there exists a constant λ depending on α and y (and therefore on μ and q) such that the error of the approximation method described above is bounded by*

$$|y(x_m) - y_m| \leq \lambda m^\alpha h^2, \quad m = 0, 1, \dots, N.$$

Corollary 5.1.8 *Under the assumptions of Theorem 5.1.7, we have the following global error estimate for the approximation method described above:*

$$\max_{m=0,1,\dots,N} |y(x_m) - y_m| = O(h^{2-\alpha}).$$

Remark 5.1.3 *We remark here, that while the given error bounds are applicable to a number of problems, the assumption $y \in C^2[0, T]$ is quite restricting. In particular we know by Corollary 4.2.8 that in general the solution does not satisfy $y \in C^2[0, T]$, so that we have to be careful when we use the given error bounds.*

We summarize our main findings of this chapter:

Different formulation of fractional backward difference methods:

- In this chapter a different way (in comparison to Chapter 5.1.1) to transfer the idea of backward differences to the fractional case has been presented.
- The new backward difference formula is not only different in its deduction but also in its resulting formula: We have changed the representation of formula (5.11) to show that we get different sets of weights $\tilde{\omega}_{km}$ and $\hat{\omega}_{km}$ for the two backward difference formulas (5.22) and (5.24).
- We have gained a new formula (formula (5.22)) for the numerical solution of equations of the type

$$f(x, y) = -\mu y + q(x)$$

with some $\mu > 0$ and some continuous function q . The error of formula (5.22) for this special kind of right-hand side behaves as $O(h^{2-\alpha})$ for $0 < \alpha < 1$.

The following chapter will expand the idea of fractional order backward differences derived in Chapter 5.1.1 to higher-order methods corresponding to higher-order methods of the classical backward difference methods for ordinary differential equations. In particular we will give a more detailed error and stability analysis for the given methods which will include the special case described in Chapter 5.1.1 (and in parts the one described in this Chapter).

5.1.3 Lubich's fractional backward difference methods

In this Chapter we are going to construct higher-order backward difference methods for fractional order differential equations based on their classical counterparts. We prepared the analytical background in Chapter 4.3, where we considered fractional linear multistep methods, to which fractional backward difference methods form a subset. The idea of fractional linear multistep methods was first presented by a number of papers by Lubich [93, 95, 96, 97] and for a special type of Volterra integral equations numerically implemented by Hairer, Lubich and Schlichte in [63]. Lubich's results apply for many important kinds of fractional linear multistep method as shown in Chapter 4.3, but in this chapter we will especially be interested in the generalization of classical backward difference methods to the fractional case, which we will denote as *Lubich's fractional backward difference methods*. We start our investigation of Lubich's fractional backward difference methods by briefly repeating the analytical results needed to describe it:

In Theorem 4.3.15 the following statement was proven: Given an Abel-Volterra integral equation of the form

$$(5.26) \quad y(x) = f(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} K(x, t, y(t)) dt, \quad x \in [0, X], \quad \alpha > 0$$

with a bounded kernel $K(x, t, y(t))$ and a given forcing function $f(x)$, the fractional linear multistep method defined by

$$(5.27) \quad y_m = f(x_m) + h^\alpha \sum_{j=0}^m \omega_{m-j} K(x_m, x_j, y(x_j)) + h^\alpha \sum_{j=0}^s w_{m,j} K(x_m, x_j, y(x_j)),$$

gives an approximation to the true solution $y(x_m)$, whose error satisfies

$$(5.28) \quad \max_{0 \leq m \leq N} |y_m - y(x_m)| = O(h^{p-\varepsilon}),$$

with a small $\varepsilon \geq 0$. In (5.27) the convolution weights ω_m are given by the generating function

$$\omega^\alpha(\zeta) = \left(\frac{\sigma(1/\zeta)}{\rho(1/\zeta)} \right)^\alpha$$

where (ρ, σ) are the characteristic polynomials of a classical linear multistep method and the starting weights $\omega_{m,j}$ are given by the linear equation system

$$(5.29) \quad \sum_{j=0}^s w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma+\alpha)} m^{\alpha+\gamma} - \sum_{j=1}^m \omega_{m-j} j^\gamma, \quad \gamma \in \mathcal{A}$$

with

$$(5.30) \quad \mathcal{A} = \{\gamma = k + j\alpha; k, j \in \mathbb{N}_0, \gamma \leq p-1\}, \quad \text{card } \mathcal{A} = s+1.$$

Furthermore in Theorem 4.2.3 we have seen how the fractional differential equations (5.1) and (5.2) can be transferred to Abel-Volterra integral equations. More precisely, the

fractional differential equation of Caputo type (5.2) can be understood as Abel-Volterra integral equation

$$(5.31) \quad y(x) = T_{n-1}[y; 0](x_m) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt$$

where the forcing function $T_{n-1}[y; 0](x_m)$ is completely defined by the initial conditions of (5.2) and the kernel $K(t, x, y(x)) = f(x, y(x))$ is given by the right-hand side of (5.2).

Finally, in Example 2.2.2 we have seen that the classical backward difference method of order p possesses the generating function

$$(5.32) \quad \omega(\zeta) = \sum_{k=0}^p \omega_k \zeta^k = \sum_{k=1}^p \frac{1}{k} (1-\zeta)^k.$$

With these results we have carried together everything needed to describe Lubich's fractional backward difference method completely:

Theorem 5.1.9 *Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Lubich's fractional backward difference method of order $p \in \{1, \dots, 6\}$ for a fractional differential equation of Caputo type (5.2) rewritten as Abel-Volterra integral equation (5.31) is given by*

$$(5.33) \quad y_m = T_{n-1}[y; 0](x_m) + h^\alpha \sum_{j=0}^m \omega_{m-j} f(x_j, y(x_j)) + h^\alpha \sum_{j=0}^s w_{m,j} f(x_j, y(x_j))$$

for $m = 1, \dots, N$, where the convolution weights ω_m are given by the generating function

$$\omega^\alpha(\zeta) = \left(\sum_{k=1}^p \frac{1}{k} (1-\zeta)^k \right)^{-\alpha}$$

and the starting weights $\omega_{m,j}$ are given by the solution of the linear equation system (5.29). Equation (5.33) gives an approximation of order $O(h^{p-\varepsilon})$ with a small $\varepsilon \geq 0$ for all fixed mesh points x_m .

The use of backward difference formulas for Abel-Volterra integral equations is well known [95, 96, 98] and even implemented in a FORTRAN code for a special type of Abel-Volterra integral equations in [64]. But even though we could use Theorem 5.1.9 directly as numerical method to solve fractional differential equations, it is more reasonable to use a slightly different method given by

Theorem 5.1.10 *Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. Lubich's fractional backward difference method of order $p \in \{1, \dots, 6\}$ for a fractional differential equation of Caputo type (5.2) is given by*

$$(5.34) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{j=0}^{m-1} \omega_{m-j} y(x_j) - \sum_{j=0}^s w_{m,j} y(x_j) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$$

for $m = 1, \dots, N$, where the convolution weights ω_m are given by the generating function

$$(5.35) \quad \omega^\alpha(\zeta) = \left(\sum_{k=1}^p \frac{1}{k} (1-\zeta)^k \right)^\alpha$$

and the starting weights $\omega_{m,j}$ are given by the solution of the linear equation system

$$(5.36) \quad \sum_{j=0}^s w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)} m^{\gamma-\alpha} - \sum_{j=1}^m \omega_{m-j} j^\gamma, \quad \gamma \in \mathcal{A}$$

with \mathcal{A} as defined in (5.30). The weights $w_{m,j}$ are of order $O(m^{-\alpha-1})$ and the error satisfies $O(h^{p-\varepsilon})$ with a small $\varepsilon \geq 0$ for all fixed mesh points x_m .

Proof: This theorem is a simple reformulation of Theorem 4.3.12 (with α replaced by $-\alpha$), where we utilized the structure of the solution of the fractional differential equation as described in Corollary 4.2.8. \square

Remark 5.1.4 a) The restriction of order $p \in \{1, \dots, 6\}$ is based on the fact that the classical backward difference methods are stable only up to order $p = 6$ (see e.g. [70]), which is a necessary condition of Theorem 4.3.11 for the stability of the fractional backward difference method.

b) The 'small value ε ' in Theorem 5.1.9 and Theorem 5.1.10 is given by equation (4.87), i.e.

$$\varepsilon = p - \alpha - \min\{\gamma = k + j\alpha, k, j \in \mathbb{N}_0, \gamma > p - 1\}$$

and thus in particular is zero for $\alpha = q/(q+1)$ with $q \in \mathbb{N}$.

c) The advantage of formula (5.36) compared to formula (5.33) is mainly founded by the fact that in formula (5.36) the convolution and starting weights are multiplied with (already computed) points of the solution, whereas in formula (5.33) they are multiplied with the right-hand side of the differential equation, which may complicate the algorithm, especially if the right-hand side is nonlinear.

d) Both Theorem 5.1.9 and Theorem 5.1.10 can be formulated for fractional differential equations of Riemann-Liouville type. The formulas (5.33) and (5.36) change correspondingly, i.e. instead of the Taylor-polynomial T_{n-1} we need to write \hat{T}_{n-1} as defined in equation (5.12). But for Riemann-Liouville type equations the Remark 5.1.1 b) still holds.

e) Theorem 5.1.9 and Theorem 5.1.10 choose the starting weights in a particular way; they ensure that the set of basis functions $b(x) = x^{k+j\alpha}$, $k + j\alpha \in \mathcal{A}$ are integrated (or respectively differentiated) exactly. In Chapter 4.3 we have seen that these basis functions are exactly the low order terms of the asymptotic expansion. These low order terms pose the principal problem of higher-order methods, since they are not accounted for in the fractional linear multistep method consisting of the convolution part alone.

With Theorem 5.1.10 we have established a generalization of the classical backward difference methods to the fractional case. We have not yet addressed in detail the computation of the two sets of weights ω_m and $w_{m,j}$ and the fact that formula (5.36) cannot be solved step-by-step for the first $s+1$ mesh points. However, the computation of the two sets of weights can be done seemingly straight forward (since the convolution weights are given by a generating function and the starting weights by a regular linear equation system) and for the first $s+1$ mesh points we may simply solve the first $s+1$ equations in formula (5.36) simultaneously as a nonlinear equation system with a proper Newton-type method. We summarize the stated results as follows:

Fractional backward difference methods of order $p \in \{1, \dots, 6\}$:

- A (non)linear fractional order differential equation of Caputo type with $\alpha > 0$ can be solved by formula (5.36), where in the first $s + 1$ steps a (non)linear equations system and in each step $m = s + 1, \dots, N$ a (non)linear equation has to be solved.
- The error at any fixed mesh point is given by $O(h^{p-\varepsilon})$ with small $\varepsilon \geq 0$ where the choice of p and the order α of the fractional differential equation determine the parameter s , given by $\text{card}\mathcal{A} - 1$ with \mathcal{A} defined in (5.30), as well as the weights ω_m and $w_{m,j}$ given by the generating function (5.35) and the linear equation system (5.36) respectively.
- In case of homogenous initial conditions, formula (5.36) without the term $h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$ describes a fractional backward difference methods of order p for fractional differential equations of Riemann-Liouville and Caputo type.

On a closer look at the implementation of this method two problems will arise. On the one hand the seemingly unproblematic computation of the two sets of weights is much more complicated than one might expect by the results so far. On the other hand the simple approach to solve the first $s + 1$ points of the solution as nonlinear equation system will have much greater impact than one would suspect. Due to their importance, we will dedicate Chapter 5.3 to these *pitfalls*. But before that, we look at a completely different method to gain access to a numerical solution of problems of type (5.1) and (5.2), which will become useful in our investigations of the pitfalls in Chapter 5.3.

5.2 Generalized Taylor expansion and Adomian's decomposition method

There are a number of different numerical approaches to solve Abel-Volterra integral equations (and thus fractional order differential equations) apart from the fractional backward difference formulas. Some of them are also based on fractional multistep methods, as we will see for example in Chapter 5.4, others are based on so called *collocation methods* (see e.g. [19, 83] and the references given there), where the singularity at the left end of integration is dealt with by non equispaced meshes, or *product integration*, where the kernel is approximated by a polynomial (spline) and the integral is evaluated by quadrature methods (see e.g. [83, 112] and the references given there or Chapter 5.1.2 for a basic understanding).

In this chapter we want to explore two other numerical methods for the solution of Abel-Volterra integral equations and in particular fractional order differential equations, which are well known for ordinary differential equations and are usually denoted as *Taylor series expansion technique* and *Adomian's Decomposition method*. The results of this chapter will not only present a different numerical method itself, but more importantly give us useful

results for the implementation of Lubich's fractional backward difference methods, which we will investigate in the next chapter.

In this chapter we will focus our attention again on fractional differential equations of Caputo type (5.2), i.e. Abel-Volterra integral equations of the form

$$(5.37) \quad y(x) = g(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt,$$

where $g(x)$ is defined by

$$g(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} b_k.$$

In particular we will work with regular initial value problems, where the functions $g(x)$ and $f(x, y(x))$ are assumed to possess a representation by a convergent Taylor series developed at 0 or $(0, g(0))$ respectively, i.e.

$$(5.38) \quad g(x) = \sum_{k=0}^{\infty} g_k x^k, \quad f(x, y(x)) = \sum_{\ell, m=0}^{\infty} f_{\ell, m} x^{\ell} (y - g_0)^m,$$

or corresponding finite series of sufficiently high order. By Theorem 4.2.7 and Corollary 4.2.8 we know that the solution $y(x)$ will exist on a certain interval $[0, X]$ and can be written as the expansion

$$(5.39) \quad y(x) = \sum_{k=0}^K \sum_{j=0}^J c_{kj} x^{k+j\alpha} + y^*(x),$$

where the parameters K and J depend on the precise smoothness properties of f and g , while y^* is smooth on $[0, X]$ and satisfies $y^*(x) = o(x^{K+J\alpha})$ as $x \rightarrow 0$. If f and g are sufficiently smooth, the first summands in the expansion (5.39) correspond to the set of basis functions which are evaluated exactly by Lubich's fractional backward difference formula (5.34) by choosing the starting weights accordingly. In other words the exponents of x in the first summands in the sum of (5.39) are given by the set \mathcal{A} defining the starting weights in Lubich's fractional backward difference method, i.e.

$$(5.40) \quad \mathcal{A} = \{\gamma = k + j\alpha; k, j \in \mathbb{N}_0, \gamma \leq p-1\}, \quad \text{card } \mathcal{A} = s+1.$$

We will present two methods to compute the asymptotic expansion of the solution of equation (5.2) and (5.37) near the starting point. The asymptotic expansion itself will then give a numerical method (by only computing a finite part of the expansion). More importantly these methods will show us a way to get hold of the lower order terms in (5.39) efficiently. We will use this fact in Chapter 5.3 to simplify Lubich's fractional backward difference method.

First we look at a generalization of the Taylor expansion technique for ordinary differential equations described in [65, Ch I.8] followed by a description of Adomian's decomposition method. Particularly with regard to their use in the upcoming section we will focus our attention to gain the expansion for the low-order terms in the expansion (5.39), i.e. the terms described by the sum. After their description we will compare both methods and point out their advantages and disadvantages in practical computations followed by two examples, which will clarify the theoretical description of the two methods.

Generalized Taylor expansion:

Let $0 < \alpha < 1$ and for stability reasons $p \in \{1, 2, \dots, 6\}$ (see Remark 5.1.4 a)). Furthermore let $0 = \gamma_0 < \gamma_1 < \dots < \gamma_s = p - 1$ be the ordered elements of the set \mathcal{A} given in (5.40). We define $D_j = D_*^{\gamma_j - \gamma_{j-1}}$ for $j = 1, \dots, s$, and denote by \mathcal{D}_k the following concatenation: $\mathcal{D}_k = D_k D_{k-1} \dots D_1$. The succession of the concatenation is important since the Caputo operators are not associative, i.e. in general applying the operator \mathcal{D}_k will produce a different result than applying $D_*^{\gamma_k}$.

We substitute the Ansatz

$$y(x) = \sum_{j=0}^s c_j x^{\gamma_j} + y^*(x)$$

in equation (5.37) but omit the term $y^*(x)$ in the following calculations because its order is higher than γ_s and we are only interested in terms up to order x^{p-1} . The integral on the right-hand side of (5.37) is of order $O(x^\alpha)$ and thus we get $c_0 = b_0$. Applying \mathcal{D}_1 on both sides of equation (5.37) yields

$$\begin{aligned} \Gamma(\alpha + 1)c_1 + O(x^\kappa) &= f(x, y(x)) \\ \Leftrightarrow \Gamma(\alpha + 1)c_1 + O(x^\kappa) &= f(0, c_0) + O(x^\kappa) \end{aligned}$$

where $\kappa > 0$ (in this case $\kappa = \alpha$ or $\kappa = 1 - \alpha$). Thus by matching the coefficients we get $c_1 = f(0, c_0)/\Gamma(\alpha + 1)$. Similarly by applying the operator \mathcal{D}_k for $k = 2, \dots, s$ we get

$$\begin{aligned} \mathcal{D}_k \left(\sum_{j=0}^s c_j x^{\gamma_j} \right) &= \mathcal{D}_k \left(b_0 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt \right) \\ \Leftrightarrow \Gamma(\gamma_k + 1)c_k + O(x^\kappa) &= \mathcal{D}_k \left(\frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt \right) \\ \Leftrightarrow \Gamma(\gamma_k + 1)c_k + O(x^\kappa) &= D_k D_{k-1} \dots D_2 f(x, y(x)), \end{aligned}$$

and by matching coefficients

$$(5.41) \quad c_k = \frac{1}{\Gamma(\gamma_k + 1)} [D_k D_{k-1} \dots D_2 f(x, y(x))]_{x=0}.$$

In particular the term $[D_k D_{k-1} \dots D_2 f(x, y(x))]_{x=0}$ is only dependent on the already known coefficients c_0, c_1, \dots, c_{k-1} . Note that formula (5.41) is the appropriate generalization of formula (8.18) in [65, Ch. I.8]. The case $\alpha > 1$ can be treated similarly: The first n steps reproduce the initial conditions and from the $(n+1)$ st step the integral part can be treated as in the case of $0 < \alpha < 1$.

With this algorithm we can compute all coefficients c_j , $j = 0, \dots, s$, which gives us complete knowledge of the sum in equation (5.39). We use this later to simplify Lubich's fractional backward difference method. Of course, depending on the differentiability properties of $f(x, y(x))$, the described method can be used to compute more terms of the expansion (5.39) and thus give a numerical solution by itself. Before going into more details on the implementation of those ideas, we give a different but closely related method to gain knowledge of the asymptotic expansion, which is based on an algorithm which recently became known as Adomian's Decomposition method, described in [3].

Adomian's decomposition method:

This method is based on the idea to construct the solution of the Abel-Volterra integral equation (5.37) as infinite sum of basis solutions $y_i(x)$, $i = 0, 1, \dots$, i.e.

$$y(x) = \sum_{i=0}^{\infty} y_i(x) = g(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} \sum_{i=0}^{\infty} {}_f A_i(t) dt,$$

where the ${}_f A_i(t)$ are the so called *Adomian polynomials*. This decomposition method is an explicit scheme, defined by

$$(5.42) \quad y_0(x) = g(x) \quad y_{i+1}(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} {}_f A_i(t) dt, \quad i = 0, 1, 2, \dots,$$

where the Adomian polynomials ${}_f A_i(x)$ are given by

$$(5.43) \quad {}_f A_i(x) = \left[\frac{1}{i!} \frac{d^i}{d\lambda^i} f \left(x, \sum_{j=0}^i \lambda^j y_j \right) \right]_{\lambda=0}.$$

(The functions y_j , $j = 0, \dots, i$ are dependent from x , but for clarity of the notation we simply write y_j instead of $y_j(x)$ from now on). Even if one cannot use the infinite scheme, it is possible to obtain a finite expansion corresponding to the differentiability properties of $f(x, y(x))$. This finite expansion contains again all information on the low order terms we need in the upcoming chapter in the implementation of Lubich's fractional backward difference method.

We present here an explicit formula for the Adomian polynomials ${}_f A_i$. In order to achieve this we will use Faà di Bruno's formula (see Theorem 2.1.9) yielding:

Theorem 5.2.1 (Adomian's decomposition method - via Faà di Bruno's formula) *Under assumption (5.38) the formula (5.43) is given as*

$$(5.44) \quad {}_f A_i(x) = \frac{1}{i!} \sum_{\ell=0}^{\infty} \sum_{m=1}^i f_{\ell,m} x^{\ell} \sum m! (1!y_1)^{b_1} (2!y_2)^{b_2} \dots (i!y_i)^{b_i}$$

where the third sum is over all partitions of $\{1, 2, \dots, i\}$ and for each partition, m is its number of blocks and b_i is the number of blocks with exactly i elements.

Example 5.2.1 *Let us consider the fourth Adomian polynomial. The partitions of $\{1, 2, 3, 4\}$ were already given in Example 2.1.1, so that we can calculate ${}_f A_4(x)$ directly:*

$$\begin{aligned} {}_f A_4(x) &= \frac{1}{4!} \sum_{\ell=0}^{\infty} \sum_{m=1}^4 f_{\ell,m} x^{\ell} \sum m! (1!y_1)^{b_1} (2!y_2)^{b_2} \dots (4!y_4)^{b_4} \\ &= \frac{1}{24} \sum_{\ell=0}^{\infty} x^{\ell} \left[f_{\ell,1} 1! (4!y_4)^1 + 4f_{\ell,2} 2! (1!y_1)^1 (3!y_3)^1 + \right. \\ &\quad \left. 3f_{\ell,2} 2! (2!y_2)^2 + 6f_{\ell,3} 3! (1!y_1)^2 (2!y_2)^1 + f_{\ell,4} 4! (1!y_1)^4 \right] \\ &= \sum_{\ell=0}^{\infty} x^{\ell} \left[f_{\ell,1} y_4 + 2f_{\ell,2} y_1 y_3 + f_{\ell,2} y_2^2 + 3f_{\ell,3} y_1^2 y_2 + f_{\ell,4} y_1^4 \right] \end{aligned}$$

Proof: (of Theorem 5.2.1) Using assumption (5.38) in formula (5.43) and the fact that $y_0 = g_0$ we get

$$(5.45) \quad {}_f A_i(x) = \left[\frac{1}{i!} \frac{d^i}{d\lambda^i} \sum_{\ell, m} f_{\ell, m} x^\ell \left(\sum_{j=1}^i \lambda^j y_j \right)^m \right]_{\lambda=0}$$

Defining

$$f(\lambda) = \sum_{j=1}^i \lambda^j y_j, \quad \text{and} \quad g(f(\lambda)) = \left(\sum_{j=1}^i \lambda^j y_j \right)^m$$

we find first that

$$f^{(r)}(\lambda) \Big|_{\lambda=0} = r! y_r, \quad r = 1, 2, \dots, i$$

and furthermore that

$$g^{(r)}(x)|_{x=f(\lambda)} = m(m-1)(m-2) \cdots (m-r+1) (f(\lambda))^{m-r}, \quad r = 1, 2, \dots$$

Noting that the term $f(\lambda)$ in the last equation evaluated at $\lambda = 0$ will vanish for all cases unless $m = r$ we immediately see that only the derivatives up to $r = i$ are non-zero. Thus the last equation simplifies to

$$g^{(r)}(f(\lambda)) = r(r-1)(r-2) \cdots (r-r+1) = r! = m!, \quad m = 1, 2, \dots, i.$$

Applying Faà di Bruno's formula to equation (5.45) we thus get formula (5.44). \square

In any practical application or if f and g are not differentiable often enough, the sum over ℓ in (5.44) will terminate after a finite number of terms. An inspection of (5.44) shows that according to (5.40) it is enough to use $\ell \leq p-1$ to gain all knowledge we will need in Chapter 5.3 to enhance Lubich's fractional backward difference formula of order p .

Remark 5.2.1 *It is of historical interest to note that the idea of Adomian's Decomposition method can be found in a number of articles by O. Perron [113, 114, 115, 116] published 1919 and 1920.*

Comparison of the two methods:

The generalized Taylor technique gives the correct expansion up to an order which is specified a-priori, while the Adomian series gives the asymptotic expansion and additional terms of higher order. This behaviour is reflected by the fact that Adomian's method requires stronger differentiability assumptions. The generalized Taylor technique incorporates all theoretically possible coefficients and can therefore introduce artificial computational complexity. Adomian's method does not possess this drawback, so the structure of the solution is easier to recognize and the computations are often simplified significantly. We will now look at two examples (one linear, one nonlinear) to clarify the structure of both methods

Example 5.2.2 *Consider the linear fractional differential equation*

$$(5.46) \quad D_*^\alpha y(x) = x + y(x), \quad y(0) = 1, \quad 0 < \alpha < 1$$

or equivalently the Volterra integral equation

$$y(x) = 1 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} (t + y(t)) dt$$

The analytical solution to this problem is given by

$$y(x) = E_\alpha(x^\alpha) + \frac{1}{\Gamma(1-\alpha)} \int_0^x (x-t)^{-\alpha} \left(E_\alpha(t^\alpha) - \frac{t^\alpha}{\Gamma(\alpha+1)} - 1 \right) dt,$$

where $E_\alpha(x)$ is the Mittag-Leffler function (see Definition 3.4.1). This can be written as the sum of the two convergent series, i.e.

$$(5.47) \quad y(x) = \sum_{j=0}^{\infty} \frac{x^{j\alpha}}{\Gamma(j\alpha+1)} + \sum_{i=1}^{\infty} \frac{x^{1+i\alpha}}{\Gamma(i\alpha+2)}.$$

If we want to use the fractional backward difference formula of order 4 and $\alpha = 0.7$ for example, we need 11 starting weights corresponding to the set \mathcal{A} given by

$$(5.48) \quad \mathcal{A} = \{0, 0.7, 1, 1.4, 1.7, 2, 2.1, 2.4, 2.7, 2.8, 3\}$$

We first calculate the expansion utilizing the generalized Taylor technique. The operator \mathcal{D}_{10} is given by

$$(5.49) \quad \begin{aligned} \mathcal{D}_{10} &= D_{10} D_9 D_8 D_7 D_6 D_5 D_4 D_3 D_2 D_1 \\ &= D_*^{0.2} D_*^{0.1} D_*^{0.3} D_*^{0.3} D_*^{0.1} D_*^{0.3} D_*^{0.3} D_*^{0.4} D_*^{0.3} D_*^{0.7} \end{aligned}$$

We substitute the Ansatz

$$y(x) = \sum_{j=0}^s c_j x^{\gamma_j} + y^*(x),$$

but we will omit $y^*(x)$ in the following calculation because its order is higher than 3. We get $c_0 = 1$ from the initial condition and $c_1 = 1/\Gamma(1.7)$ by our observation in the above description of the technique. By formula (5.41) the coefficient c_2 is given by

$$\begin{aligned} c_2 &= \frac{1}{\Gamma(2)} \left[D_2 \left(x + \sum_{j=0}^{10} c_j x^{\gamma_j} \right) \right]_{x=0} \\ &= \frac{1}{\Gamma(2)} \left[\frac{\Gamma(2)}{\Gamma(1.7)} x^{0.7} + \sum_{j=1}^{10} \frac{\Gamma(\gamma_j+1)}{\Gamma(\gamma_j+1-0.3)} c_j x^{\gamma_j-0.3} \right]_{x=0} = 0. \end{aligned}$$

Similarly c_3 and c_4 are computed by

$$\begin{aligned} c_3 &= \frac{1}{\Gamma(2.4)} \left[D_3 D_2 \left(x + \sum_{j=0}^{10} c_j x^{\gamma_j} \right) \right]_{x=0} \\ &= \frac{1}{\Gamma(2.4)} \left[\frac{\Gamma(2)}{\Gamma(1.3)} x^{0.3} + \sum_{j=1}^{10} \frac{\Gamma(\gamma_j+1)}{\Gamma(\gamma_j+1-0.7)} c_j x^{\gamma_j-0.7} \right]_{x=0} = \frac{1}{\Gamma(2.4)}, \end{aligned}$$

$$\begin{aligned}
c_4 &= \frac{1}{\Gamma(2.7)} \left[D_4 D_3 D_2 \left(x + \sum_{j=0}^{10} c_j x^{\gamma_j} \right) \right]_{x=0} \\
&= \frac{1}{\Gamma(2.7)} \left[\frac{\Gamma(2)}{\Gamma(1)} x^0 + \sum_{j=2}^{10} \frac{\Gamma(\gamma_j + 1)}{\Gamma(\gamma_j + 1 - 1)} c_j x^{\gamma_j - 1} \right]_{x=0} = \frac{1}{\Gamma(2.7)}.
\end{aligned}$$

In the same way we can compute the values for c_j ($j = 5, \dots, 11$) and we get

$$\begin{aligned}
c_5 &= 0, & c_6 &= \frac{1}{\Gamma(3.1)}, & c_7 &= \frac{1}{\Gamma(3.4)}, \\
c_8 &= 0, & c_9 &= \frac{1}{\Gamma(3.8)}, & c_{10} &= 0.
\end{aligned}$$

Thus we have computed the asymptotic expansion for all lower terms, i.e the solution is given by

$$\begin{aligned}
y(x) &= 1 + \frac{1}{\Gamma(1.7)} x^{0.7} + \frac{1}{\Gamma(2.4)} x^{1.4} + \frac{1}{\Gamma(2.7)} x^{1.7} + \frac{1}{\Gamma(3.1)} x^{2.1} \\
&\quad + \frac{1}{\Gamma(3.4)} x^{2.4} + \frac{1}{\Gamma(3.8)} x^{2.8} + y^*(x)
\end{aligned}$$

where $y^*(x) = O(x^{3.1})$. These are obviously the first terms of the exact solution (5.47) and thus we have obtained the exact structure of the low order terms of the solution.

Next we are going to produce the asymptotic expansion with Adomian's method. The given problem (5.46) is linear and thus ${}_f A_i = y_i$ follows for $i \geq 1$. Therefore, Adomian's method yields for the case $\alpha = 0.7$:

$$\begin{aligned}
y_0 &= 1, \\
y_1 &= \frac{x^{0.7}}{\Gamma(1.7)} + \frac{x^{1.7}}{\Gamma(2.7)}, \\
y_2 &= \frac{x^{1.4}}{\Gamma(2.4)} + \frac{x^{2.4}}{\Gamma(3.4)}, \\
y_3 &= \frac{x^{2.1}}{\Gamma(3.1)} + \frac{x^{3.1}}{\Gamma(4.1)}, \\
y_4 &= \frac{x^{2.8}}{\Gamma(3.8)} + \frac{x^{3.8}}{\Gamma(4.8)}.
\end{aligned}$$

The summation of y_0, \dots, y_4 yields the correct expansion up to order $x^{3.1}$. This finite Adomian series is not the correct expansion up to $x^{3.8}$, because the $x^{3.5}$ -term will be included in the not yet computed basis solution y_5 .

Example 5.2.3 Consider the nonlinear fractional differential equation

$$(5.50) \quad D_*^\alpha y(x) = x^2 + y^2(x), \quad y(0) = b_0, \quad 0 < \alpha < 1$$

or equivalently the Volterra integral equation

$$y(x) = b_0 + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} (t^2 + y^2(t)) dt.$$

This is obviously a regular problem, we can rewrite (5.50) to

$$D_*^\alpha y(x) = x^2 + (y(x) - b_0)^2 + 2b_0(y - b_0) + b_0^2, \quad y(0) = b_0, \quad 0 < \alpha < 1.$$

Choosing the same parameters as in the linear example, i.e. $p = 4$ and $\alpha = 0.7$ we get again \mathcal{A} as in (5.48) and \mathcal{D}_{10} as in (5.49). We get $c_0 = b_0$ from our initial condition and $c_1 = b_0^2/\Gamma(1.7)$ from our observation of Section 3. The next coefficients c_j are computed as follows:

$$\begin{aligned} c_2 &= \frac{1}{\Gamma(2)} \left[D_2 \left(x^2 + \left(\sum_{j=1}^{10} c_j x^{\gamma_j} \right)^2 + 2b_0 \sum_{j=1}^{10} c_j x^{\gamma_j} + b_0^2 \right) \right]_{x=0} \\ &= \frac{1}{\Gamma(2)} \left[O(x^{1.7}) + O(x^{1.1}) + O(x^{0.4}) \right]_{x=0} = 0, \\ c_3 &= \frac{1}{\Gamma(2.4)} \left[D_3 D_2 \left(x^2 + \left(\sum_{j=1}^{10} c_j x^{\gamma_j} \right)^2 + 2b_0 \sum_{j=1}^{10} c_j x^{\gamma_j} + b_0^2 \right) \right]_{x=0} \\ &= \frac{1}{\Gamma(2.4)} \left[O(x^{1.3}) + O(x^{0.7}) + \Gamma(1.7) 2b_0 c_1 + O(x^{0.7}) \right]_{x=0} = \frac{2}{\Gamma(2.4)} b_0^3. \end{aligned}$$

The coefficients c_4 and c_5 vanish, as can be easily seen.

$$\begin{aligned} c_6 &= \frac{1}{\Gamma(3.1)} \left[D_6 \dots D_2 \left(x^2 + \left(\sum_{j=1}^{10} c_j x^{\gamma_j} \right)^2 + 2b_0 \sum_{j=1}^{10} c_j x^{\gamma_j} + b_0^2 \right) \right]_{x=0} \\ &= \frac{1}{\Gamma(3.1)} \left[(x^{0.6}) + \Gamma(2.4) c_1^2 + O(x^{0.7}) + \Gamma(2.4) 2b_0 c_3 + O(x^{0.7}) \right]_{x=0} \\ &= \left(\frac{\Gamma(2.4)}{\Gamma(3.1)\Gamma^2(1.7)} + \frac{4}{\Gamma(3.1)} \right) b_0^4. \end{aligned}$$

The coefficients c_7, \dots, c_{10} can be calculated in the same way. They are:

$$\begin{aligned} c_7 &= 0, & c_8 &= \frac{2}{\Gamma(3.7)}, \\ c_9 &= \left(\frac{4b_0\Gamma(3.1)}{\Gamma(1.7)\Gamma(2.4)\Gamma(3.8)} + \frac{4}{\Gamma(3.8)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.8)} \right) b_0^4, & c_{10} &= 0. \end{aligned}$$

For Adomian's decomposition method we use the Faà di Bruno's formula as described in Section 3.2. First we note, that the Taylor coefficients of the right-hand side of (5.50) are all zero apart from $f_{0,0} = b_0^2$, $f_{0,1} = 2b_0$, $f_{0,2} = 1$ and $f_{2,0} = 1$. Thus we get the first Adomian

polynomials as

$$\begin{aligned}
 {}_fA_0(x) &= \sum_{\ell=0}^{\infty} f_{\ell,0}x^{\ell} = b_0^2 + x^2, \\
 {}_fA_1(x) &= \sum_{\ell=0}^{\infty} f_{\ell,1}x^{\ell}y_1 = 2b_0y_1, \\
 {}_fA_2(x) &= \sum_{\ell=0}^{\infty} f_{\ell,1}x^{\ell}y_2 + f_{\ell,2}x^{\ell}y_1^2 = 2b_0y_2 + y_1^2, \\
 {}_fA_3(x) &= \sum_{\ell=0}^{\infty} f_{\ell,1}x^{\ell}y_3 + 2f_{\ell,2}y_1y_2 + f_{\ell,3}y_1^3 = 2b_0y_3 + 2y_1y_2.
 \end{aligned}$$

and the first basis solution as

$$\begin{aligned}
 y_0 &= b_0, \\
 y_1 &= J^{\alpha} [b_0^2 + x^2] = \frac{b_0^2}{\Gamma(1.7)}x^{0.7} + \frac{2}{\Gamma(3.7)}x^{2.7}, \\
 y_2 &= J^{\alpha} \left[2b_0 \left(\frac{b_0^2}{\Gamma(1.7)}x^{0.7} + \frac{2}{\Gamma(3.7)}x^{2.7} \right) \right] \\
 &= \frac{2b_0^3}{\Gamma(2.4)}x^{1.4} + \frac{4b_0}{\Gamma(4.4)}x^{3.4}, \\
 y_3 &= J^{\alpha} \left[2b_0 \left(\frac{2b_0^3}{\Gamma(2.4)}x^{1.4} + \frac{4b_0}{\Gamma(4.4)}x^{3.4} \right) + \left(\frac{b_0^2}{\Gamma(1.7)}x^{0.7} + \frac{2}{\Gamma(3.7)}x^{2.7} \right)^2 \right] \\
 &= \left(\frac{4}{\Gamma(3.1)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.1)} \right) b_0^4x^{2.1} + \left(\frac{8}{\Gamma(5.1)} + \frac{4\Gamma(4.4)}{\Gamma(1.3)\Gamma(3.7)\Gamma(5.1)} \right) b_0^2x^{4.1} \\
 &\quad + \left(\frac{4\Gamma(6.4)}{\Gamma^2(3.7)\Gamma(7.1)} \right) x^{6.1}, \\
 y_4 &= J^{\alpha} [y_3 + 2y_1y_2] \\
 &= x^{2.8} \frac{\Gamma(3.1)}{\Gamma(3.8)} b_0^4 \left(\frac{4b_0}{\Gamma(1.7)\Gamma(2.4)} + \frac{4}{\Gamma(3.1)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.1)} \right) + \\
 &\quad x^{4.8} \frac{\Gamma(5.1)}{\Gamma(5.8)} b_0^2 \left(\frac{8b_0}{\Gamma(3.7)\Gamma(2.4)} + \frac{8b_0}{\Gamma(1.7)\Gamma(4.4)} + \frac{8}{\Gamma(5.1)} + \frac{4\Gamma(4.4)}{\Gamma(1.3)\Gamma(3.7)\Gamma(5.1)} \right) + \\
 &\quad x^{6.8} \frac{\Gamma(7.8)}{\Gamma(8.5)} \left(\frac{16b_0}{\Gamma(3.7)\Gamma(4.4)} + \frac{4\Gamma(6.4)}{\Gamma^2(3.7)\Gamma(7.1)} \right)
 \end{aligned}$$

Thus we get from both methods the expansion of the lower terms:

$$y(x) = b_0 + \frac{b_0^2}{\Gamma(1.7)}x^{0.7} + \frac{2b_0^3}{\Gamma(2.4)}x^{1.4} \left(\frac{4}{\Gamma(3.1)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.1)} \right) b_0^4x^{2.1} + \frac{2}{\Gamma(3.7)}x^{2.7}$$

$$+ \left(\frac{4b_0\Gamma(3.1)}{\Gamma(1.7)\Gamma(2.4)\Gamma(3.8)} + \frac{4}{\Gamma(3.8)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.8)} \right) b_0^4 x^{2.8} + y^*(x),$$

where $y^*(x) = O(x^{3.1})$.

Both methods described in this chapter can be used to obtain the asymptotic expansion of the solution of Abel-Volterra integral equations. Thus these methods can be considered by themselves as a type of numerical method to solve fractional order differential equations, if we only develop the expansion up to a finite parameter (as we did in the examples). However, a more important benefit of the described method lies in a different fact: Both methods produce the lower order terms in the expansion of the exact solution, which coincide with the basis functions in Lubich's higher order method. Thus, depending on the given right-hand side of a differential equation, we may not have to account for all exponents of the solution as given in Corollary 4.2.8, but only for those, who exist in the expansion of the exact solution as produced by either of the stated methods. We will discuss a numerical scheme, which utilizes this result in the next chapter. Before summarizing the results of this section, we state some additional remarks on the two described methods:

Remark 5.2.2 a) We note that it may not be easy to calculate the Taylor coefficients of the right-hand side of problem (5.2), which are necessary to apply both described methods. This aspect also holds for the classical integer order case as described in [65, Ch. 1.8] and is in fact the major drawback of these methods. Nevertheless, useful results of the integer order case dealing with this problem can be applied directly to the fractional case.

b) There exist fast formulas to compute the indices of the Faà di Bruno's formula described in Theorem 2.1.9 (see e.g. [75]). While these calculations are tediously done by hand they are nevertheless quickly obtained by a computer algorithm.

c) If we are just interested in the exponents of the low order terms in expansion (5.39) and not their exact factors we can use the Adomian polynomials given by the Faà di Bruno's formula and the knowledge of the Taylor coefficients of the right hand side of the given problem (5.2) to quickly calculate the possible elements of the set \mathcal{A} . (Note: If we do not calculate the factors exactly, we might miss simplifications, which arise because different components contributing to a specific coefficient can cancel each other, i.e. the element 2.5 in the case $\alpha = 0.5$ could have emerged from any of the first five Adomian polynomials. Of course, if all Taylor coefficients have the same sign for example, such a cancellation cannot occur.) Furthermore we can state some simple rules, e.g. "If the right-hand side of equation (5.2) with $0 < \alpha < 1$ is solely dependent on $y(x)$ only multiples of α can be present in the exact expansion of the solution (5.39)", which can easily be seen by the structure of the Adomian polynomials.

Methods to obtain the asymptotic expansion of the solution of a fractional differential equation:

- Given a fractional differential equation whose right-hand side is sufficiently differentiable, we can obtain the asymptotic expansion of the exact solution by either the generalized Taylor technique or by Adomian's decomposition method.
- Adomian's decomposition method requires higher differentiability of $f(x, \cdot)$ than the generalized Taylor technique to compute the asymptotic expansion up to a fixed order.
- Both methods, while tedious done by hand, can be efficiently implemented in a computer algorithm following the description of the two methods.
- For certain right-hand sides the structure of the Adomian polynomials enables us to draw conclusions about the structure of the expansion prior to its exact computation.

5.3 Numerical computation of fractional backward difference methods and its pitfalls

In this chapter we want to take a closer look at the implementation of the higher-order backward difference method based on Lubich's work described in Chapter 5.1.3. In particular we are not only interested in the analytical results, but rather in an implementation of these results and its possible pitfalls. Some of the results in this chapter repeat the findings of a recent article [35].

We focus our attention once again on the case of fractional differential equations of Caputo type, i.e.

$$(5.51) \quad D_*^\alpha y(x) = f(x, y(x)), \quad D^k y(0) = b_k \quad (k = 0, 1, \dots, n-1), \quad n = \lceil \alpha \rceil.$$

We know that for a given equispaced mesh $0 = x_0, x_1, \dots, x_N = X$ a numerical solution of this equation on the interval $[0, X]$ is given by formula

$$(5.52) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{j=0}^{m-1} \omega_{m-j} y(x_j) - \sum_{j=0}^s w_{m,j} y(x_j) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$$

for $m = 1, \dots, N$ and $y_0 = b_0$, whose error behaves as $O(h^{p-\varepsilon})$ with a small $\varepsilon \geq 0$. In this formula the only unknowns are the convolution weights ω_m , which are given by their generating function

$$(5.53) \quad \omega^\alpha(\zeta) = \left(\sum_{k=1}^p \frac{1}{k} (1 - \zeta)^k \right)^\alpha,$$

and the starting weights $\omega_{m,j}$, which are given by the solution of the linear equation system

$$(5.54) \quad \sum_{j=0}^s w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)} m^{\gamma-\alpha} - \sum_{j=1}^m \omega_{m-j} j^\gamma, \quad \gamma \in \mathcal{A},$$

where the set \mathcal{A} is dependent of α and p and defined by

$$(5.55) \quad \mathcal{A} = \{\gamma = k + j\alpha; k, j \in \mathbb{N}_0, \gamma \leq p-1\}, \quad \text{card} \mathcal{A} = s+1.$$

For an implementation of these results we therefore have to investigate the following questions:

- (In which way) can the convolution weights be computed accurately and efficiently from their generating function (5.53)?
- (In which way) can the starting weights be computed accurately and efficiently from the linear system (5.54)?
- (In which way) can formula (5.52) be solved and how do the answers of the other questions affect the accuracy of formula (5.52)?

All these questions seem rather simple and in fact we have given simple answers to them at the end of Chapter 5.1.3. We now want to give more detailed answers.

Since formula (5.52) needs both convolution and starting weights and the equation system of the starting weights demands knowledge of the convolution weights, we begin our investigation with the computation of the weights ω_m .

5.3.1 Computation of the convolution weights ω_m

As it turns out the question of an efficient and accurate computation of the convolution weights is fortunately the least complicated problem we have to deal with and can be quickly answered by the following theorem:

Theorem 5.3.1 *The convolution weights ω_m , $m = 0, 1, \dots$ of a fractional linear multistep method ω can be computed recursively by the formula*

$$(5.56) \quad \omega_m = \frac{1}{mu_0} \sum_{j=0}^{m-1} [\alpha(m-j) - j] \omega_j u_{m-j},$$

if the generating function $\omega(\zeta)$ of the underlying linear multistep method $\omega = (\sigma, \rho)$ is analytic. The values u_m , $m = 0, 1, \dots$ in (5.56) denote the Taylor expansion coefficients of the generating function $\omega(\zeta)$ of the underlying non-fractional linear multistep method $\omega = (\sigma, \rho)$.

Proof: The proof of this theorem is based on Automatic Differentiation (see e.g. [127]). Given an analytic function $f(x)$, we can represent it by

$$(5.57) \quad f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k = \sum_{k=0}^{\infty} f_k x^k,$$

where the constants f_k denote the Taylor coefficients of f . Similarly the first derivative of the function $f(x)$ can also be represented by its Taylor polynomial expansion:

$$(5.58) \quad f'(x) = \sum_{k=1}^{\infty} \frac{f^{(k)}(0)}{(k-1)!} x^{k-1} = \sum_{k=0}^{\infty} (k+1) f_{k+1} x^k.$$

The last expression of equation (5.58) gives us therefore a formula for the Taylor coefficients of the first derivative of the function $f(x)$ using only the Taylor coefficients of the function $f(x)$ itself. Another well known formula for generating Taylor coefficients is Leibniz' formula for a function $f(x) = g(x)h(x)$ given by

$$(5.59) \quad f_n = \sum_{k=0}^n g_{n-k} h_k.$$

With these results we have everything we need in order to prove formula (5.56):

For a given function $f(x) = [g(x)]^\alpha$ with an arbitrary constant $\alpha \in \mathbb{R}$ we take the first derivative and get

$$(5.60) \quad f'(x)g(x) = \alpha f(x)g'(x).$$

We consider both sides of this equation as functions, generate the corresponding m th Taylor coefficients on each side using the Leibniz rule (5.59) and get

$$(5.61) \quad \sum_{k=0}^m g_{m-k} f'_k = \alpha \sum_{k=0}^m g'_{m-k} f_k.$$

Exploiting formula (5.58) we can rewrite (5.61) to

$$\sum_{k=0}^m g_{m-k} (k+1) f_{k+1} = \alpha \sum_{k=0}^m (m-k+1) g_{m-k+1} f_k.$$

By extracting the last summand of the left-hand side we first get

$$(m+1)f_{m+1}g_0 + \sum_{k=0}^{m-1} g_{m-k}(k+1)f_{k+1} = \alpha \sum_{k=0}^m (m-k+1)g_{m-k+1}f_k,$$

and by modifying the rest of the sum

$$(m+1)f_{m+1}g_0 = \alpha \sum_{k=0}^m (m-k+1)g_{m-k+1}f_k - \sum_{k=0}^m g_{m-k+1}k f_k.$$

Combining the two sums and division by $(m+1)g_0$ finally yields

$$f_{m+1} = \frac{1}{(m+1)g_0} \sum_{k=0}^m [\alpha(m-k+1) - k] g_{m-k+1} f_k.$$

□

Remark 5.3.1 a) We first note that the stated result in Theorem 5.3.1 is not new, in fact it can be derived with some work [109, Thm. 4.1.15] from the J. C. P. Miller formula, (see e.g. [71, pp. 41-42]).

b) The generating function $\omega(\zeta)$ for the p -th order classical backward difference formula is a polynomial of order $p + 1$. This means that only the Taylor coefficients u_0, u_1, \dots, u_p in the formula (5.56) are non-zero. Hence for weights ω_k with $k \geq p + 1$, the sum in (5.56) reduces to

$$(5.62) \quad w_k = \frac{1}{ku_0} \sum_{j=k-(p+1)}^{k-1} [\alpha(k-j) - j] \omega_j u_{k-j},$$

and therefore at most $p + 1$ summands are needed for each convolution weight ω_m , $m = 0, 1, \dots$

c) The use of the Fast Fourier Transform is often stated as an efficient way to compute the convolution weights (see e.g. [64, §3.]). However, a closer look often reveals that the described methods require some special structure of α (e.g. in [64, §3.] to be a unit fraction) to be able to apply Fast Fourier Transforms successfully. Of course, this is added to the fact that Fast Fourier Transforms will only perform at its best, if the number of weights are a power of 2. More precisely, if the number of weights are given by $N = 2^q$, $q \in \mathbb{N}$, the Fast Fourier Transform computes the weights in less than $\phi(N) = 51N \log_2(4N)$ multiplications (see e.g. [72, pp. 520-521]), while the J. C. P. Miller formula needs $\phi(N) = N^2$ multiplications. Thus only in the case that α is a unit fraction and the number of weights is $N = 2^q$, with $q > 9$, $q \in \mathbb{N}$ the Fast Fourier Transform should be used instead of the J. C. P. Miller formula.

d) Last we note that formula (5.61) does not exhibit any problematic behavior so that we can reasonably assume that an implementation in a computer algorithm will produce the weights close to machine precision.

With Theorem 5.3.1 and in particular formula (5.62) we have found an efficient and accurate way to compute the convolution weights ω_m . The next item on our agenda is the computation of the starting weights $w_{m,j}$ which is much more complicated and in fact will lead to the biggest drawback of fractional backward difference formulas.

5.3.2 Computation of the starting weights $w_{m,j}$

A closer look at the linear equation system (5.54) reveals the following: The coefficient matrix $(a_{ij}) = (j^{\gamma_i}), \gamma_i \in \mathcal{A}$ of (5.36) is an exponential Vandermonde matrix (which is a generalized Vandermonde matrix with real exponents, see e.g. [132]). Thus it is regular, assuring a unique solution for the starting weights $w_{m,j}$. But it is also ill-conditioned which points out two possible problems: On the one hand we might ask under which condition we will be able to find an accurate solution of the equation system and, if we will not be able to find an accurate solution, what are the consequences of an inexact solution? The problem of finding an accurate solution is hampered even more by another aspect of system (5.36): As already remarked in [96, §4.2], the evaluation of the right-hand side of (5.54) suffers from cancellation of digits. The first of the above questions will be answered in this chapter and show that we will almost never be able to find an “exact” solution and the consequence of this fact will be addressed in Chapter 5.3.3.

While from the analytical point of view the equation system (5.54) exhibits no problems, a numerical implementation has to cope with its ill-conditioning and should exploit its special structure in a certain way.

In order to compare any method for computing the starting weights we need some sort of measure, characterizing the accuracy of the solution. This is usually achieved by comparing the *residuals* of the equation system (5.54), i.e. the value of

$$(5.63) \quad \sum_{j=0}^s w_{m,j} j^{\gamma} + \sum_{j=1}^m \omega_{m-j} j^{\gamma} - \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)} m^{\gamma-\alpha}, \quad \gamma \in \mathcal{A}.$$

This approach is also justified by the fact that in earlier works [64, 96] the condition of having a small residual is noted to be important for an accurate overall method. Furthermore in [96] it is asserted that this can happen, even if the errors in the starting weights themselves are not small.

Remark 5.3.2 *a) The importance of small residuals can mathematically be analyzed in detail from the analytical results as we will see in detail in Chapter 5.3.3. An immediate interpretation is given by the fact Lubich's fractional backward difference methods require to integrate (or respectively differentiate) the basis functions exactly as explained in Remark 5.1.4 e). Therefore, by the analytical results, they need to vanish (or in computation need to be as small as possible).*

b) The precise condition number of the coefficient matrix depends on the value of α in a very subtle way: For example, if $\alpha = 1/q$ with some integer q then it can be rewritten by an obvious change of variables in the form of a classical Vandermonde matrix which is mildly ill-conditioned. If, however, $\alpha = 1/q - \epsilon$ with some small $|\epsilon|$ and $p \geq 2$, then the set \mathcal{A} will contain the elements 1 and $q\alpha = 1 - q\epsilon$, and hence the matrix will have two almost identical columns and therefore an extremely bad condition number.

As a result of the second remark we start our investigation of the solvability of the equation system (5.54) with the apparently simplest case, where α is a unit fraction:

Björck-Pereyra algorithm for the case $\alpha = 1/q$, $q \in \mathbb{N}$:

If α is a unit fraction we can use the fact that

$$(5.64) \quad j^{\gamma} = j^{k+\ell\alpha} = j^{r\alpha} = (j^{\alpha})^r, \quad r = 0, 1, \dots, s$$

and immediately see that the coefficient matrix is a classical Vandermonde matrix. Hence an algorithm exploiting this well known structure may prove useful. Given the fact that we have to solve the system (5.54) for as many right-hand sides as mesh points in our quadrature, the use of the algorithm by Björck and Pereyra [13] to obtain the inverse of the matrix seems well suited: Their algorithm is fast, requiring only $O((s+1)^2)$ arithmetic operations to solve a linear equation system with $s+1$ variables. More importantly Higham showed in [73] that if the Björck-Pereyra algorithm is used to invert a classical Vandermonde matrix for which the defining elements are positive and monotonically ordered (which is true for our system (5.54) with substitution (5.64)) the estimate

$$(5.65) \quad |\hat{V}^{-1} - V^{-1}| \leq 5(s+1)\epsilon_M |V^{-1}| + O(\epsilon_M^2)$$

holds, where ϵ_M is the *machine precision* (see further Remark 5.3.3 c)) and \hat{V}^{-1} is the inverse of the Vandermonde matrix V computed by the algorithm. The estimate (5.65) has to be understood component wise using the modulus of matrices, defined by $|A| = (|a_{ij}|)$. The computation of the inverse of the coefficient matrix using the Björck-Pereyra algorithm needs $O((s+1)^3)$ arithmetic operations. But since our system will in general be small and more importantly the error bound (5.65) is independent of the condition number of the Vandermonde matrix V , this algorithm seems appropriate for the given problem.

However, while theoretically the Björck-Pereyra algorithm seems to be well fitted for our problem, the practical implementation fails, because the estimate (5.65) is dependent on the entries of the exact inverse V^{-1} whose absolute values are getting exceedingly large in our cases due to the structure of the exponential Vandermonde system.

So apparently even the least problematic case (in terms of only mild ill-conditioning of the coefficient matrix) exhibits severe problems in calculating the starting weights $\omega_{m,j}$, even though we exploited the special structure of the coefficient matrix. So instead of using our knowledge of the problematic behaviour and the special structure of the equation system we might use a standard solver for the linear equation system.

Standard solver for the case $\alpha \in \mathbb{R}$:

Completely disregarding our initial remarks about the ill-conditioning of the coefficient matrix and the cancellation of digits on the right-hand side, we might use a standard solver for the regular equation system (5.54). A typical equation system solver will first apply an LU decomposition on the coefficient matrix and then solve the two corresponding systems recursively. Since we have a regular problem an implementation of this method will produce some sort of solution, which we then could use - more or less blindly - as the “correct” weights in formula (5.52).

A different approach to tackle the equation system is the use of a non-stationary iterative solver suited for our problem.

Generalized Minimum Residual method (GMRES) for the case $\alpha \in \mathbb{R}$:

The *Generalized Minimum Residual method* (GMRES) by Saad and Schultz [140] seems to be the most promising iterative solver (for further reading we refer to the book [139] by Saad). This assessment is based on the fact that we are primarily concerned with obtaining an approximate solution to (5.54) for which the residual is small (see also Chapter 5.3.3). GMRES has the property that the norm of the residual is minimized over the current Krylov subspace at each iteration. In addition, the non-Hermitian nature of the system rules out many of the cheaper alternatives and its denseness means that GMRES will be less expensive to apply than methods, such as Conjugate Gradient Squared (CGS), that require more than one matrix-vector multiplication at each step (see [61, §5.7]). In exact arithmetic GMRES will converge to the exact solution in no more than $s+1$ iterations, but its convergence behavior in a finite-precision implementation is currently not well-understood, particularly for ill-conditioned problems, so we cannot predict in advance whether or not the method will provide solutions to (5.54) with suitably small residuals. A disadvantage of this approach compared with either direct solution by LU decomposition or computation of the inverse matrix is that the iteration has to be repeated for each different right-hand side, rather than using the readily computed LU factors or inverse matrix to solve each system. Thus we expect this method to be considerably more expensive in terms of computer time.

We investigated both standard GMRES and the slightly modified GMRES solver by Walker [145] where the Householder transformation is used for the computation of the Krylov space instead of the modified Gram-Schmidt orthonormalization. The justification of this concept lies in the fact that the modified Gram-Schmidt orthonormalization can fail to perform well if the vectors of the Krylov space are not sufficiently independent (as they are especially in cases where the choice of α results in two almost identical columns). Indeed, if $Q = \{q_0, q_1, \dots, q_{k-1}\}$ denotes the orthonormalized basis of the Krylov space S computed by the modified Gram-Schmidt method with floating point arithmetic of precision ϵ_M , then the following estimate holds (see Björck [12]):

$$(5.66) \quad Q^T Q = I + E, \quad \|E\|_2 \approx \epsilon_M \kappa_2(S).$$

Here $\kappa_2(S)$ denotes the (2-norm) condition number of the matrix S . However using the Householder transformations yields under the same notation as in (5.66) the following estimate (see Björck [12]):

$$(5.67) \quad Q^T Q = I + E, \quad \|E\|_2 \approx \epsilon_M,$$

which is independent of the condition number $\kappa_2(S)$ of the original basis of the Krylov space and thus it may give better results for our system.

Comparison of the three methods for solving equation system (5.54):

For the paper [35] an experiment for the calculation of starting weights using the four methods described above (counting the two different gmres methods each as one) was carried out. All calculations were done in Matlab Version 6.5 in double precision. For the standard solver (denoted by “lu” in the tables below) the Matlab backslash operator “\” was used, which in fact applies an LU decomposition on the coefficient matrix and then solves the corresponding systems. Secondly a Matlab implementation of the the Björck-Pereyra algorithm (“bp”) for inverting the Vandermonde matrix was written and tested for the cases where α was a unit fraction. At last two tests using the GMRES algorithm were carried out: (a) the Matlab *gmres* function (“gmres”), which uses the Gram-Schmidt orthonormalization; and (b) an implementation using the method of [145, Algorithm 2.2] (“gmresh”) was written in Matlab to check the GMRES algorithm with Householder transformation. In both cases the full (i.e. not re-started) GMRES without preconditioning and with a stopping tolerance of $1e-16$ (which was never, in practice, achieved) was used.

The following tables give the results of these experiments. The notation $1.02(-4)$ stands for $1.02 \cdot 10^{-4}$, etc. The average residuals of the first 1000 starting weights for the different methods are given for various choices of α . The best value for each choice of α is marked in bold.

The different values of α above are only an extract of the number of different values, for which the different methods were tested. We repeat here the conclusion which were drawn from these results in [35]:

- The Björck-Pereyra algorithm should not be used for the computation of the starting weights. However, a different algorithm exploiting the special structure of the exponential Vandermonde matrix may give better results in the future.
- The LU decomposition method gives a slightly worse result for the starting weights than either of the GMRES methods. However, the computational time of the LU

α	$\frac{1}{10}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$
lu	1.02(-4)	5.61(-6)	2.59(-7)	3.66(-11)	2.31(-14)
bp	1.34(33)	9.79(2)	5.00(-3)	9.59(-8)	4.95(-12)
gmres	1.01(-5)	2.57(-6)	4.39(-7)	3.75(-11)	1.56(-14)
gmresh	3.85(-6)	2.63(-6)	1.33(-7)	2.26(-11)	1.27(-13)

Table 5.1: Average residuals for various numerical methods for the exponential Vandermonde system (5.54) with α being a unit fraction.

α	0.49	0.51	$\frac{2}{3}$	$\frac{4}{5}$	$\frac{9}{10}$
lu	1.12(-5)	1.38(-8)	9.87(-13)	1.43(-11)	5.98(-12)
gmres	1.75(-6)	6.92(-9)	7.82(-13)	5.04(-12)	8.66(-12)
gmresh	1.76(-6)	6.93(-9)	3.11(-12)	2.76(-11)	4.01(-11)

Table 5.2: Average residuals for various numerical methods for the exponential Vandermonde system (5.54) with α not being a unit fraction.

decomposition is far below that of the GMRES methods. Therefore, it has advantages when attempting to implement a fast scheme.

- Both GMRES methods perform equally well. Each one has certain values of α where it is advantageous compared to the other one. However, the Householder transformation needs more computation time than the Gram-Schmidt orthonormalization. In cases where the “best” results are needed and computation time is not the most important factor, the GMRES method should be used.
- For almost all choices of α , *none* of the four methods produces starting weights which are exact to machine precision. Therefore, in general, problems will arise in using any of those weights in the quadrature as we will describe in more detail in Chapter 5.3.3.

Remark 5.3.3 *a) It is possible that the solution cost and/or the accuracy of the residuals computed using the GMRES iterations could be improved by using a preconditioner. However, some limited experiments using standard preconditioning techniques for dense matrices (e.g. incomplete LU decomposition, diagonal and band approximation, wavelet compression) have been unsuccessful and in some cases have increased both the residual norm and the computation time. Difficulties in designing an effective preconditioner for this system are to be expected, since most standard preconditioners are based on approximating the inverse of the system matrix, which we know cannot be done accurately in this case. Moreover, although theoretical results are not available for GMRES, it is known that, for ill-conditioned systems, preconditioning is ineffective in improving the accuracy of other Krylov subspace methods, such as Conjugate Gradients (see [61]).*

b) Apart from the value of the residual itself, the actual distribution of the residual over the different starting weights between using a standard solver or a GMRES method for the starting weight computation was ascertained in [35]: In Figure 5.1 the starting weights

as well as their residuals for the case $\alpha = \frac{1}{10}$ and 10000 nodes for the two different system solvers are shown.

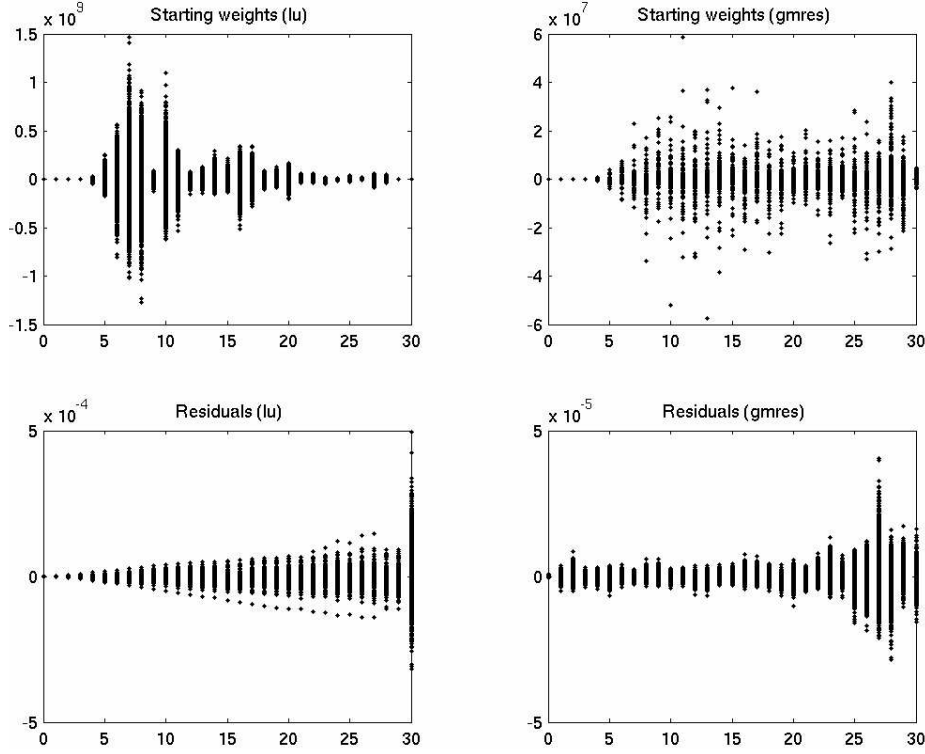


Figure 5.1: Starting weights and residuals for $\alpha = \frac{1}{10}$ and $N = 10000$ computed by LU decomposition and GMRES method, respectively. Each dot represents one starting weight or residual. All 31 starting weights for the nodes $N = 1, 2, \dots, 10000$ are shown.

c) Apart from the described four methods, there exists another way to ensure, that the residuals in the computation of the starting weights are small (enough): The way a computer handles any number is that it does not use the exact number x but rather its floating point representation $fl(x)$. The maximum error between the exact number and the floating point is given by

$$\frac{|fl(x) - x|}{|x|} \leq \epsilon_M,$$

where ϵ_M is the machine precision, which is usually either single ($\epsilon_M = 2^{-24} \approx 10^{-7}$) or double ($\epsilon_M = 2^{-53} \approx 10^{-16}$) precision. (see IEEE Computer Society (1985), IEEE Standard for Binary Floating-Point Arithmetic, IEEE Std 754-1985) Roughly said single precision retains 7 and double precision 16 correct digits in the floating point representation of any number x .

Today's computers work internally with double precision and thus mathematical operations are optimized in computer programs to deal with double precision numbers. Neverthe-

less it is possible to use “better” machine precision using software implementations to retain more digits of the exact number in floating point representation. Over the last years a number of quad precision or variable precision packages for different programming languages have been developed, which could be used to obtain “small residuals” for the equation system (5.54).

Therefore, a number of tests were carried out using a software package by Knut Petras (GMP-XSC: An Interval-Multiple-Precision Library based on GNU Multiple Precision (GMP)) to carry out the computation of the starting weights in variable machine precision. The test showed that we can obtain residuals with roughly double precision carrying out the calculation solving the linear equation system in quad or higher machine precision. But the computation time for the weights can then take up days - even weeks - which is to be expected using software packages in order to work in higher machine precision. However, since the starting weights are independent of the stepsize h this approach is in theory feasible to construct a database with small starting weights and then use these precalculated weights in formula (5.52).

d) We focused our attention on the problematic coefficient matrix and not on the cancellation of digits on the right-hand side. While the latter also leads to problematic behaviour, its influence on the starting weights themselves is less severe. Nevertheless we will see in the following chapter, in particular in Figure 5.3, that it can complicate the mentioned problem in its own way.

e) In general the magnitude of the residual gives a strong indication on how well Lubich’s backward difference method will perform. In particular we can not expect errors smaller than the residuals for general types of problems.

The above results clearly show that we usually can not expect to gain correct starting weights or even starting weights having small residuals (an exception e.g is the most commonly treated choice of $\alpha = 1/2$, where we retain almost machine precision, see Table 5.1).

The next question is therefore in which way the wrongly calculated starting weights will affect the numerical solution of the fractional order differential equation using Lubich’s fractional backward difference formula (5.52).

5.3.3 Solving the fractional differential equations by formula (5.52)

In order to investigate Lubich’s fractional backward difference method further we rewrite formula (5.52) to

$$(5.68a) \quad y_m = F_m + \sum_{j=s+1}^{m-1} \omega_{m-j} y(x_j), \quad m = 1, \dots, N, \quad y_0 = b_0$$

with

$$(5.68b) \quad F_m = h^\alpha f(x_m, y_m) - \sum_{j=0}^s \omega_{m-j} y(x_j) - \sum_{j=0}^s w_{m,j} y(x_j) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m).$$

This representation of formula (5.52) partitions the problem into two separate parts. For the first $s + 1$ steps we have to solve a nonlinear equation system with $s + 1$ equations

and $s + 1$ variables. This nonlinear equation system can be solved with Newton's method. The needed *starting values* y_0, \dots, y_s can either be obtained from additional knowledge of the given problem (such as an asymptotic expansion near the origin) or, if no additional information exists, can all be set to the initial value $y_0 = b_0$. For $m = s + 1, \dots, N$ we have to solve a nonlinear equation to obtain the numerical solution y_m . This can be achieved by a suitable fixed point method.

Remark 5.3.4 *Since the solution y_0 is known from the (first) initial condition we only have to solve a nonlinear equation system with s equations and unknowns. This fact is reflected by a closer look at the starting weights $w_{0,j}$, which are all zero except $w_{0,0} = 1$.*

In view of the findings in the previous Chapter 5.3.2 the following questions need to be addressed:

- (In which way) do the possibly inaccurate starting weights influence formula (5.68a)?
- (In which way) do the possibly inexact starting values influence formula (5.68a)?

We start the investigation of these two questions with an inspection of the starting weights, more precisely we look at the magnitude of the starting weights from a theoretical and computational point of view:

Investigation of the magnitude of the starting weights $w_{m,j}$:

In earlier papers [64, 94, 96] the condition $|w_{mj}| = O(m^{-\alpha-1})$ (or respectively $O(m^{\alpha-1})$ for Abel-Volterra integral equations) is given as an important condition on the starting weights for stability of the numerical scheme. Baker and Derakhshan (see e.g. [11]) point out that the starting weights will satisfy this condition for a range of numerical schemes, including Lubich's fractional backward difference method. However they assume that the Vandermonde system has been solved exactly. Therefore, it is reasonable for us to consider the values of $|w_{mj}|$ as m varies as one way of testing the likely performance of Lubich's fractional backward difference method. In the following discussion the starting weights have been calculated using Matlab's backslash operator "`\`". While we have seen in Chapter 5.3.2 that a different solver might produce slightly better results, all investigated solvers inherited the generic problem of not accurately computing the starting weights for different choices of α . The behaviour in the following figures are therefore valid for the slightly better solvers as well, as we have tested in numerous experiments.

We present first a figure (Figure 5.2) showing how the calculated starting weights vary for up to 60 grid points and $\alpha = \frac{1}{2}$. From Table 5.1 we know that the residuals of the starting weights are calculated almost to machine precision. Figure 5.2 illustrates the phenomenon that we would hope to see and reflects the good performance of Lubich's backward difference method in this case, as was for example ascertained in [64].

More surprising is the next figure (Figure 5.3). Here we present the starting weights for $\alpha = \frac{1}{2}$ but for much larger numbers of grid points. We draw attention to the way in which suddenly the method that is known to perform really well for small numbers of grid points exhibits behaviour that would suggest a poor approximate solution for a larger number of grid points. We shall see below that this is indeed what will happen.

Now we present a figure similar to Figure 5.2 for $\alpha = \frac{1}{10}$ (Figure 5.4). For clarity we only show the 15th starting weight. From Table 5.1 we know that now the residuals of the

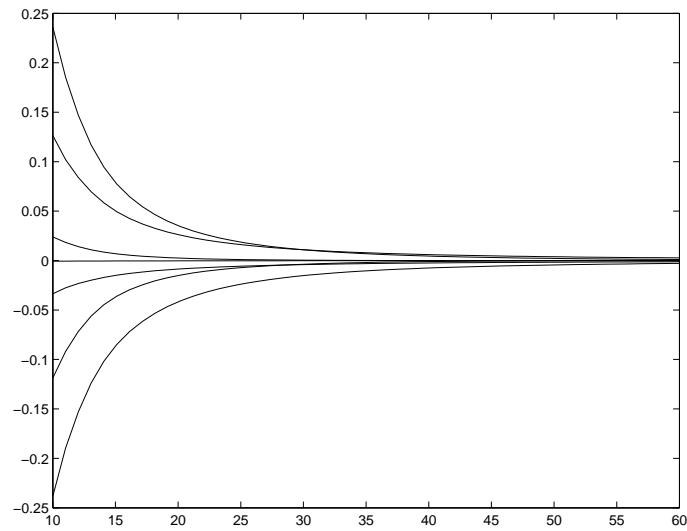


Figure 5.2: Starting weights for $\alpha = \frac{1}{2}$ and $n = 10, 11, \dots, 60$. Each line represents one column of starting weights.

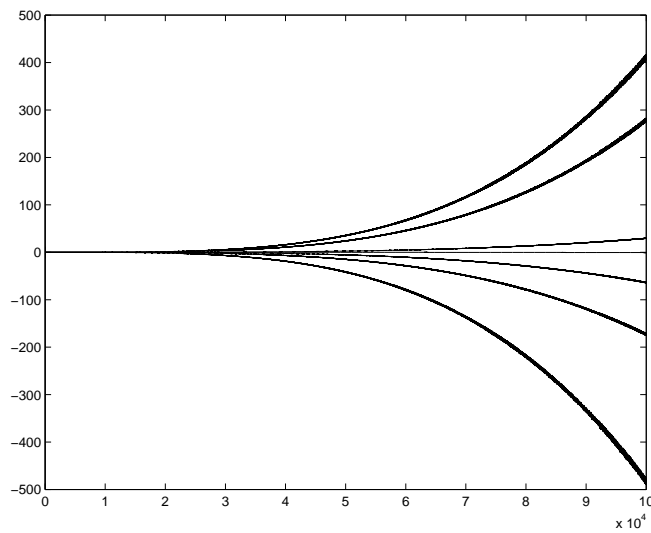


Figure 5.3: Starting weights for $\alpha = \frac{1}{2}$ and $n = 1, 2, \dots, 100000$. Each line represents one column of starting weights.

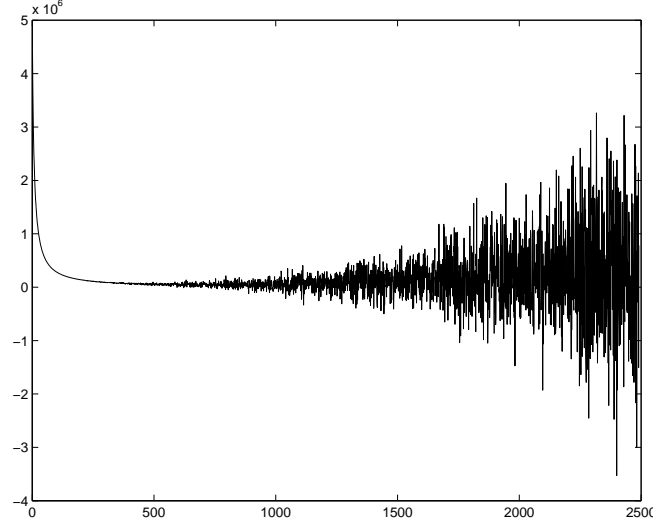


Figure 5.4: Starting weight for $\alpha = \frac{1}{10}$ and $n = 10, 11, \dots, 2500$. Only the graph of the 15th starting weight is drawn. The behaviour is typical of all 31 starting weights.

starting weights do not even reach single machine precision and thus we expect a different behaviour of the magnitude of the starting weights; While the magnitude of the starting weight decreases in the beginning as one would expect from the theory, the explosion we have seen for the case $\alpha = \frac{1}{2}$ occurs for $\alpha = \frac{1}{10}$ much sooner. In addition the behavior itself becomes chaotic. Similar behavior is observed for all 31 starting weights.

The figures we have produced here are representative for any choice of α . Depending on the magnitude of the residuals of the starting weights the blowup of the starting weights happens earlier or later. But even for the case $\alpha = 1/2$ for which we know that the residual is as close to machine precision as we could hope for, we get problematic behaviour, which will influence the whole numerical scheme. We will now give a detailed analysis of this problem:

Analysis of errors arising from starting weights and starting values:

In this section we will address both aforementioned questions, i.e. we will discuss the errors in solutions of formula (5.68a) based on errors in the starting weights and starting values. This time we approach the problem from a more theoretical viewpoint.

We assume we use Lubich's fractional backward difference method with s starting values (see Remark 5.3.4). We propose to solve the fractional differential equation over the interval $[0, X]$ where $X = Nh$ for some fixed $h > 0$.

The basic idea is as follows: we assume that the *exact* starting weights w_{mj} and convolution weights ω_{m-j} would be recorded in an $(N+1) \times (N+1)$ matrix A according to

$$(5.69) \quad A = \left(\begin{array}{c|c} I_s & 0 \\ \hline A_{21} & A_{22} \end{array} \right)$$

where I_s is an $s \times s$ identity matrix, A_{21} is the $(N+1-s) \times s$ matrix with $(A_{21})_{ij} = w_{s+i,j} + \omega_{s+i-j}$ and A_{22} is the square $(N+1-s)$ matrix with $(A_{22})_{ij} = \omega_{i-j}$ for $j \leq i$ and 0 otherwise. In practice we have perturbed weights leading to a matrix of the form $A + B$ where B takes the special form

$$(5.70) \quad B = \left(\begin{array}{c|c} 0 & 0 \\ \hline B_{21} & 0 \end{array} \right)$$

where B_{21} is the $(N+1-s) \times s$ matrix containing the errors in the starting weights $(B_{21})_{ij} = (w_{s+i,j} - \tilde{w}_{s+i,j})$. This highlights the fact that only the starting weights contain errors.

The *exact* starting values are assumed to be stored as the first s elements in a solution vector $y \in \mathbb{R}^{N+1}$ and the errors in the starting values are assumed to be stored in the first s elements of the vector $e \in \mathbb{R}^{N+1}$.

Now we are in a position to formulate our calculations in terms of the matrices A, B and the vectors y, e : the approximate solution described in formula (5.68a) is given by successive multiplication of vector y by the matrix $h^\alpha A$. Each successive multiplication by the matrix $h^\alpha A$ corresponds to evaluation of the next step in the convolution integral (starting from step s). In total we need to pre-multiply by $h^\alpha A$ a total of $N-s+1$ times to complete the solution over $[0, X]$. Thus we wish to calculate

$$(5.71) \quad J = (h^\alpha A)^{N+1-s} y.$$

In fact, when we take the inevitable errors into account, we will actually evaluate

$$(5.72) \quad \tilde{J} = (h^\alpha (A + B))^{N+1-s} (y + e)$$

so the errors introduced by the starting values and starting weights we calculated are given by the expression $\tilde{J} - J$.

Lubich's fractional backward difference method defined the starting weights in A in such a way that the method integrates *exactly* a set of s functions (see also Chapter 4.3 and 5.1.3). Each of these functions can be sampled at the values $0, h, 2h, 3h, \dots, (s-1)h$ to give a vector in \mathbb{R}^s . It is simple to see that the set of s vectors of dimension s defined in this way spans \mathbb{R}^s . We extend each of these s -dimensional vectors to an $(N+1)$ -dimensional vector by concatenating $N+1-s$ zeros in the last components to give us s linearly independent vectors that we shall call v_1, v_2, \dots, v_s .

By construction of the vectors v_i , we can see that constants α_j, β_j can be found so that $y = \beta_1 v_1 + \dots + \beta_s v_s$ and $e = \beta_1 v_1 + \dots + \beta_s v_s$.

This shows (by linearity) that successive multiplication by the matrix $h^\alpha A$ evaluates exactly both the propagation of the values in y (which we want) and the propagation of the values in e (which we do not want).

Now we can turn our attention to the effect of multiplication by the matrix $h^\alpha B$. As we constructed B it consists of the errors in the starting weights which we evaluated in accordance with the methods of Chapter 5.3.2. In their paper [64], the authors say that the *residuals* in the calculation of the starting weights (see (5.63)) need to be small. They assert (see also [96]) that this can happen even when the errors in the starting weights themselves are not very small.

Now we can see that the residuals to which they refer are the same as the values obtained by multiplying rows of B by vectors v_j . Therefore, the accuracy of the approximation of $A^{N+1-s} y$ by $(A + B)^{N+1-s} (y + e)$ hinges on the values of $B^\ell v_j$ for each vector v_j .

We recall that Baker and Derakhshan [11] have shown that, for the numerical methods of interest to us, the weights w_{mj} satisfy

$$(5.73) \quad \sup_{0 \leq j \leq m} |w_{mj}| = O(m^{\alpha-1}) \text{ as } m \rightarrow \infty.$$

It follows that $\|A\|_1 = O(N^\alpha)$ and $\|h^\alpha A\|_1 = O(1)$. Thus we see that the calculation of the solution using the *exact* starting weights is *stable with respect to small errors in the starting values*.

We can readily obtain an estimate for the worst case behaviour by evaluating (estimating) $\|B\|_1$. We know that $\|A + B\| + \|A\| \geq \|B\| \geq \|A + B\| - \|A\|$ (for any norm) and that $\|A\|_1 = O(N^\alpha)$. We have the matrix $A + B$ and so we can evaluate $\|A + B\|_1$ exactly. If $\|B\|_1$ is large then we know that certain combinations of v_j will be magnified by that factor. It is clear that $\|B\|_1$ will be small if and only if all the residuals are small.

The above discussion shows us that if the value $\|B\|_1$ is not small then the values $h^{\alpha\ell} B^\ell y$ and $h^{\alpha\ell} B^\ell e$ may become large. We wish to know whether they will in fact do this. For insight we turn to the *power method* for calculating eigenvalues of a square matrix based on repeatedly multiplying a starting vector by the given matrix. For the power method we see that if the starting vector is chosen randomly, there is a probability unity that the dominant eigenvalue will be found. However if the starting vector is chosen so that there is no component in the direction of the eigenvector with dominant eigenvalue then some less prominent eigenvalue will be found. The situation in our problem is exactly parallel with this. If the vector y (the starting vector) is chosen so that there is no component in the direction along which the matrix B exhibits its dominant behaviour, then the error produced by the dominant behaviour will not be visible in the solution. On the other hand, the starting errors e are likely to be random and therefore with probability unity will show up the dominant behaviour of the matrix B . In general, in the examples we have been working with (see Chapter 6.1), $h^\alpha(A + B)$ leads to an unstable solution operator with respect to small changes in the starting values.

As we will see in Chapter 6.1, the analysis of the errors arising from starting weights and starting values can be observed in typical examples. In particular the task of implementing a stable version of Lubich's fractional backward difference method of order p (at least for $4 \leq p \leq 6$) in a direct way will not be possible. Moreover, we will see that while using exact initial values in the starting vector (which in general have to be obtained from the nonlinear equation system) will lead to a good accurate solution, while putting in random starting errors destroys the accuracy. We can see how this can happen when we look at a section of the matrix of residuals. Almost all the residuals are quite small and therefore it is comparatively easy to find starting values that do not pick up the dominant (bad) behaviour. The random starting errors introduce all the dynamics of the solution.

With this analytical review of the practical implementation in mind we conclude the section on the implementation of Lubich's fractional backward difference method with a word on possible enhancements of the described implementation based on our results of Chapter 5.2.

5.3.4 Enhancements of Lubich's fractional backward difference method

In the last sections we have seen that Lubich's fractional backward difference method, while analytically convincing, exhibits severe drawbacks in practical implementation. In particular problems arise if Lubich's fractional backward difference methods of higher order are implemented, which is a direct result of having to compensate for more terms in the asymptotic expansion of the solution (see Chapter 4.3).

In Chapter 5.2 we have seen that the analytical expansion

$$y(x) = \sum_{k=0}^K \sum_{j=0}^J c_{ij} x^{k+j\alpha} + y^*(x),$$

of the exact solution can be obtained using generalized Taylor technique or Adomian's decomposition method. One important consequence is the fact that with knowledge of the exact expansion up to the term $x^{k+j\alpha}$ with $k+j\alpha \leq p-1$ we immediately know which basis functions we need to approximate exactly with Lubich's backward difference method. This is most easily comprehended by continuation of the two examples of Chapter 5.2.

Example 5.3.1 *In Example 5.2.2 we obtained*

$$\begin{aligned} y(x) = & 1 + \frac{1}{\Gamma(1.7)} x^{0.7} + \frac{1}{\Gamma(2.4)} x^{1.4} + \frac{1}{\Gamma(2.7)} x^{1.7} + \frac{1}{\Gamma(3.1)} x^{2.1} \\ & + \frac{1}{\Gamma(3.4)} x^{2.4} + \frac{1}{\Gamma(3.8)} x^{2.8} + y^*(x) \end{aligned}$$

where $y^*(x) = O(x^{3.1})$ as the asymptotic expansion of the solution for the fractional differential equation of Caputo type:

$$D_*^\alpha y(x) = x + y(x), \quad y(0) = 1, \quad 0 < \alpha < 1.$$

These are obviously the first terms of the exact solution (compare with (5.47)) and thus we have obtained the exact structure of the low order terms of the solution. The main result is that we could use this knowledge to reduce the set $\mathcal{A} = \{0, 0.7, 1, 1.4, 1.7, 2, 2.1, 2.4, 2.7, 2.8, 3\}$ corresponding to the needed starting weights to $\hat{\mathcal{A}} = \{0, 0.7, 1.4, 1.7, 2.1, 2.4, 2.8\}$ and apply Lubich's fractional convolution quadrature.

More distinctly we obtained in Example 5.2.3

$$\begin{aligned} y(x) = & b_0 + \frac{b_0^2}{\Gamma(1.7)} x^{0.7} + \frac{2b_0^3}{\Gamma(2.4)} x^{1.4} \left(\frac{4}{\Gamma(3.1)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.1)} \right) b_0^4 x^{2.1} + \frac{2}{\Gamma(3.7)} x^{2.7} \\ & + \left(\frac{4b_0\Gamma(3.1)}{\Gamma(1.7)\Gamma(2.4)\Gamma(3.8)} + \frac{4}{\Gamma(3.8)} + \frac{\Gamma(2.4)}{\Gamma^2(1.7)\Gamma(3.8)} \right) b_0^4 x^{2.8} + y^*(x), \end{aligned}$$

where $y^*(x) = O(x^{3.1})$ as the asymptotic expansion of the solution for the fractional differential equation of Caputo type:

$$D_*^\alpha y(x) = x^2 + y^2(x), \quad y(0) = b_0, \quad 0 < \alpha < 1.$$

The new set \hat{A} (A remains the same as in the first example) is therefore given as

$$\hat{A} = \{0, 0.7, 1.4, 2.1, 2.7, 2.8\}$$

and thus greatly reduces the number of needed basis functions to be compensated in Lubich's backward difference method.

These two examples indicate the general use of computing the low order terms of the exact expansion of the solution. In the first example the set of needed weights reduced from 11 to 7 and in the second example only 6 weights are needed in Lubich's fractional backward difference method instead of all eleven weights. This reduction has direct impact on the problematic Vandermonde matrix. In particular the condition of the matrix is greatly improved in both cases and thus the residuals will be smaller than in the general approach. In addition the reduced number of starting weights simplifies the nonlinear equation system, since its dimension gets reduced.

Remark 5.3.5 *a) One has to be careful, which weights need to be compensated in the fractional linear multistep method: If the fractional differential operator is discretized, the exponents in the Vandermonde matrix for the starting weights are the elements $\hat{\gamma}_k$ of \hat{A} , whereas if the integral operator is discretized, the exponents in the Vandermonde matrix are $\hat{\gamma}_k - \alpha$.*

b) With knowledge of the exact solution it may also be possible to transfer the given problem to one not requiring any starting weights at all. This can be obtained if the asymptotic expansion can be integrated in the right-hand side of the fractional differential equation in some way.

c) We have not yet produced a detailed error analysis of the proposed method, i.e. it remains to be shown that knowledge of the lower order terms in the exact expansion of the solution is sufficient to reduce the number of basis function in Lubich's fractional backward difference method. However, the proofs of Chapter 4.3 used only the knowledge of the general structure of the exact solution and thus it is stands to reason that the improved method is analytically sound.

Even though Lubich's backward difference method exhibits severe problems it can be successfully used to solve fractional order differential equations. *But* because of the stated analysis of error behaviour one has to be very careful in applying the method to any given problem. In particular one has to be aware of the magnitude of the residuals in the starting weights computation, which give a strong indication of the accuracy of the whole method. The results of this chapter can be summarized as follows:

Implementation of Lubich's fractional backward difference method:

- Formula (5.52) can be partitioned in two parts as shown in equations (5.68a) and (5.68b). The nonlinear equation system of the starting part (computing the mesh points $m = 1, \dots, s$) can be solved by Newton's method. As starting values one can use $b_0 = y_0 = y_1 = \dots = y_s$.
- The convolution weights of formula (5.52) can be computed accurate and efficiently by formula (5.56) and (5.62) respectively.
- The starting weights can be computed fast by solving the linear equation system (5.54) using a standard solver or slower, but more accurate, by applying a GMRES solver. In both cases the magnitude of the residuals (5.63) indicates the best outcome in the accuracy of formula (5.52).
- To increase the accuracy of formula (5.52), the starting weights can be computed in variable machine precession or the asymptotic expansion of the exact solution can be computed with the results of Chapter 5.2 to reduce the number of starting weights.

With this chapter we finish our investigation of fractional backward difference methods. In the next chapter we take a brief look on another numerical method, which is also based on fractional linear multistep methods, more precisely we will formulate the well known classical Adams-Moulton-Bashforth method in the fractional setting.

5.4 An Adams method

We now introduce a numerical method to solve the fractional differential equation of Caputo type based on the fractional formulation of the classical Adams-Bashforth-Moulton method. In particular we will use the formulation of the problem in Abel-Volterra integral form, i.e

$$(5.74) \quad y(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} b_k + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt.$$

This method has been introduced and briefly discussed in [39] and some more information is given in [38]. A number of additional results for a specific initial value problem are contained in [34], a detailed mathematical analysis is provided in [37], and additional practical remarks can be found in [36]. Numerical experiments and comparisons with other methods are reported in [41]. In this work we shall give a brief overview of the fractional formulation and state some of the known analytical results, based on the lecture script [33, Ch. 8].

In Example 2.2.1 we have briefly explained the Adams-type formulas for the classical case. We will now develop similar formulas for the fractional case. We assume that a unique solution of (5.74) exists on some interval $[0, X]$ and that we are interested in a numerical solution on the uniform grid $\{x_j = jh : j = 0, 1, \dots, N\}$ with some integer N

and stepsize $h = X/N$. Assuming that we have already calculated the approximations $y_j \approx y(x_j)$, $j = 1, 2, \dots, k$, the basic idea is to obtain the solution y_{k+1} by replacing the equation (5.74) with a discrete formula. We use the product trapezoidal quadrature formula to replace the integral in (5.74), where nodes x_j , $j = 0, 1, \dots, k+1$ are taken with respect to the weight function $(x_{k+1} - \cdot)^{\alpha-1}$. In other words, we apply the approximation

$$(5.75) \quad \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} g(z) dz \approx \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz,$$

where \tilde{g}_{k+1} is the piecewise linear interpolant for g with nodes and knots chosen at the x_j , $j = 0, 1, 2, \dots, k+1$. Arguing as in the proof of Lemma 5.1.5, we find that we can write the integral on the right-hand side of (5.75) as

$$(5.76a) \quad \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz = \sum_{j=0}^{k+1} a_{j,k+1} g(x_j)$$

where

$$(5.76b) \quad a_{j,k+1} = \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} \phi_{j,k+1}(z) dz$$

and

$$(5.76c) \quad \phi_{j,k+1}(z) = \begin{cases} (z - x_{j-1})/(x_j - x_{j-1}) & \text{if } x_{j-1} < z \leq x_j, \\ (x_{j+1} - z)/(x_{j+1} - x_j) & \text{if } x_j < z < x_{j+1}, \\ 0 & \text{else.} \end{cases}$$

An easy explicit calculation yields that, for an arbitrary choice of the x_j , (5.76b) and (5.76c) produce

$$(5.77a) \quad a_{0,k+1} = \frac{(x_{k+1} - x_1)^{\alpha+1} + x_{k+1}^\alpha [\alpha x_1 + x_1 - x_{k+1}]}{x_1 \alpha (\alpha + 1)},$$

$$(5.77b) \quad a_{j,k+1} = \frac{(x_{k+1} - x_{j-1})^{\alpha+1} + (x_{k+1} - x_j)^\alpha [\alpha (x_{j-1} - x_j) + x_{j-1} - x_{k+1}]}{(x_j - x_{j-1}) \alpha (\alpha + 1)} + \frac{(x_{k+1} - x_{j+1})^{\alpha+1} - (x_{k+1} - x_j)^\alpha [\alpha (x_j - x_{j+1}) - x_{j+1} + x_{k+1}]}{(x_{j+1} - x_j) \alpha (\alpha + 1)},$$

if $1 \leq j \leq k$, and

$$(5.77c) \quad a_{k+1,k+1} = \frac{(x_{k+1} - x_k)^\alpha}{\alpha (\alpha + 1)}.$$

In the case of equispaced nodes ($x_j = jh$ with some fixed h), these relations reduce to

$$(5.78) \quad a_{j,k+1} = \begin{cases} \frac{h^\alpha}{\alpha (\alpha + 1)} \left(k^{\alpha+1} - (k - \alpha)(k + 1)^\alpha \right) & \text{if } j = 0, \\ \frac{h^\alpha}{\alpha (\alpha + 1)} \left((k - j + 2)^{\alpha+1} + (k - j)^{\alpha+1} - 2(k - j + 1)^{\alpha+1} \right) & \text{if } 1 \leq j \leq k, \\ \frac{h^\alpha}{\alpha (\alpha + 1)} & \text{if } j = k + 1. \end{cases}$$

This then gives us our corrector formula (i.e. the fractional variant of the one-step *Adams-Moulton method*), which is

$$(5.79) \quad y_{k+1} = \sum_{j=0}^{n-1} \frac{x_{k+1}^j}{j!} b_j + \frac{1}{\Gamma(\alpha)} \left(\sum_{j=0}^k a_{j,k+1} f(x_j, y_j) + a_{k+1,k+1} f(x_{k+1}, y_{k+1}^P) \right).$$

The remaining problem is the determination of the predictor formula that we require to calculate the value y_{k+1}^P . The idea we use to generalize the one-step Adams-Bashforth method is the same as the one described above for the Adams-Moulton technique: We replace the integral on the right-hand side of equation (5.74) by the product rectangle rule

$$(5.80) \quad \int_0^{x_{k+1}} (x_{k+1} - z)^{\alpha-1} g(z) dz \approx \sum_{j=0}^k b_{j,k+1} g(x_j),$$

where now

$$(5.81) \quad b_{j,k+1} = \int_{x_j}^{x_{j+1}} (x_{k+1} - z)^{\alpha-1} dz = \frac{(x_{k+1} - x_j)^\alpha - (x_{k+1} - x_{j+1})^\alpha}{\alpha}.$$

This expression for weights can be derived in a way similar to the method used in the proof of Lemma 5.1.5. However, here we are dealing with a piecewise constant approximation and not a piecewise linear one, and hence we have had to replace the “hat-shaped” functions ϕ_{kj} by functions being of constant value 1 on $[x_j, x_{j+1}]$ and 0 on the remaining parts of the interval $[0, x_{k+1}]$. Again, in the equispaced case, we have the simpler expression

$$(5.82) \quad b_{j,k+1} = \frac{h^\alpha}{\alpha} ((k+1-j)^\alpha - (k-j)^\alpha).$$

Thus, the predictor y_{k+1}^P is determined by the fractional *Adams-Bashforth method*

$$(5.83) \quad y_{k+1}^P = \sum_{j=0}^{n-1} \frac{x_{k+1}^j}{j!} b_j + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} f(x_j, y_j).$$

Our basic algorithm, the fractional *Adams-Bashforth-Moulton method*, is thus completely described by equations (5.83) and (5.79) with the weights $a_{j,k+1}$ and $b_{j,k+1}$ being defined according to (5.77) and (5.81), respectively.

We state without their proof the most significant results on the error analysis of the described method, performed in [37]. The first result is based on smoothness assumptions on $D_*^\alpha y$ and given by

Theorem 5.4.1 *Let $\alpha > 0$ and assume $D_*^\alpha y \in C^2[0, X]$ for some suitable X . Then,*

$$(5.84) \quad \max_{0 \leq j \leq N} |y(x_j) - y_j| = \begin{cases} O(h^2) & \text{if } \alpha \geq 1, \\ O(h^{1+\alpha}) & \text{if } \alpha < 1. \end{cases}$$

We have seen in Chapter 4.2.1 that smoothness of $y(x)$ usually implies non-smoothness of $D_*^\alpha y$ (with the notable exception stated in Corollary 4.2.11). Thus we state as second result on the error behaviour the convergence of the described method with respect to the smoothness of y itself.

Theorem 5.4.2 Let $0 < \alpha < 1$ and assume that $y \in C^2[0, X]$ for some suitable X . Then, for $1 \leq j \leq N$ we have

$$(5.85) \quad |y(x_j) - y_j| \leq Cx_j^{\alpha-1} \times \begin{cases} h^{1+\alpha} & \text{if } 0 < \alpha < 1/2, \\ h^{2-\alpha} & \text{if } 1/2 \leq \alpha < 1, \end{cases}$$

where C is a constant independent of j and h .

Thus for all choices of $\alpha > 0$ the described method gives a convergence order of at least one if either y or $D_*^\alpha y$ is at least two times continuous differentiable on $[0, X]$. We summarize the results of this chapter as follows:

Adams-Bashforth-Moulton method for fractional differential equations:

- Given a fractional differential equation of Caputo type in Abel-Volterra integral form (5.74), we get a predictor-corrector type method by first predicting the solution at mesh point y_{k+1} by (5.83) and then correcting it with formula (5.79).
- The coefficients $a_{j,k}$ and $b_{j,k}$ of formula (5.83) and (5.79) are given for a uniform mesh by equations (5.78) and (5.82) respectively.
- The error of the Adams-Bashforth-Moulton method behaves depending on the differentiability of $D_*^\alpha y$ or y as in (5.84) or (5.85) respectively and is at least 1, if either $D_*^\alpha y$ or y is two times continuously differentiable on the interval $[0, X]$.

Before we start to investigate the described numerical methods for fractional differential equations in Chapter 6 for special examples and different applications, we take a moment to state some known ideas of improvements of the described numerical methods.

5.5 Notes on improvements

We have described several numerical methods in the last sections, ranging from different first-order backward difference methods, fractional Adams-Moulton-Bashforth method, algorithms computing the analytic expansion of Abel-Volterra integral equations up to formulation and inspection of higher-order backward difference formulas.

What we have not yet done, is to look at 'easy' ways to enhance the stated numerical methods with mathematical *ruses*. Such *ruses* are well known for the case of ordinary differential equations and can in parts be transferred to the fractional case. Moreover, the special structure of fractional operators causes complications in numerical methods not existent in the classical case, but they also open up additional ways to enhance numerical methods. In this chapter we are going to briefly introduce the ideas behind some improvements of the described numerical methods, but will not work through them in detail. We start with an improvement, which exploits the decaying memory behaviour of fractional derivatives.

The non-local character of fractional derivatives and correspondingly its memory effect are the most important properties of any fractional derivative in applications. But the non-local structure of fractional derivatives is also one reason, why numerical methods for fractional differential equations are much more costly in terms of computational time and storage requirements than their integer order counterparts. The kernel of the fractional integral (which exists in any definition of fractional derivatives) is usually sampled equally at each point of a given discretization. While analytically this is a necessity because of the fact that the whole interval in question influences the fractional derivative at any given point, in a discretization one can exploit the fading memory behaviour of the fractional derivative, as we will explain in the following two principles:

Fixed memory principle:

Podlubny [122, Ch. 7.3] introduced the so called *fixed memory principle* (also known as “*short-memory principle*”). The basic idea is that instead of using equally spaced sample points of the whole interval $[0, x]$ for fractional differentiation of a function $f(x)$, one might use the fading memory of fractional derivatives and only use a *fixed memory* $[x - L, x]$ of length L . The fading memory property can directly be observed by the definition of the finite Grünwald-Letnikov derivative

$${}_F^L D^\alpha f(x) = \frac{1}{h^\alpha} \sum_{k=0}^m (-1)^k \binom{\alpha}{k} f(x - kh), \quad m = x/h$$

where the coefficients $(-1)^k \binom{\alpha}{k}$ for sample points near the lower terminal 0 are small. Podlubny showed that the use of a fixed memory of length L in the finite Grünwald-Letnikov derivative introduces an error E to the approximation of the Riemann-Liouville derivative (independent of the full interval of integration) that satisfies

$$(5.86) \quad E < \frac{ML^{-\alpha}}{|\Gamma(1-\alpha)|}, \quad L \leq x \leq X$$

where $f(x) \leq M$ for $0 \leq x \leq X$. This inequality can also be used for determining the necessary length of fixed memory to assure a given accuracy ϵ of the given method, i.e.

$$(5.87) \quad E \leq \epsilon \quad \text{if} \quad L \geq \left(\frac{M}{\epsilon |\Gamma(1-\alpha)|} \right)^{1/\alpha}.$$

The negative effect of introducing an additional error in the approximation using a fixed memory of length L is balanced by the reduction in the number of summands in the finite Grünwald-Letnikov derivative to at most $\lceil L/h \rceil$. Furthermore it can be shown that for any given numerical method of order $O(h^p)$ one can apply the fixed memory principle by choosing L suitably (of order $O(h^{-p/\alpha})$).

As Ford and Simpson showed in [54], the suitable choice of the memory length L , assuring a type of error behaviour as in (5.86) usually will not reduce the computational effort unless the interval on which a solution is sought for is very large. In particular they showed that using the finite Grünwald-Letnikov derivative with fixed memory of length L to discretize the Caputo derivative of order $0 < \alpha < 1$ yields an error of the form

$$(5.88) \quad E \leq \frac{M}{|\Gamma(2-\alpha)|} (x^{1-\alpha} - L^{1-\alpha}), \quad M = \sup_{t \in (0, x)} |y'(t)|$$

which is not independent of the interval of integration. Thus for any given error bound $\epsilon > 0$ one has to choose L such that

$$(5.89) \quad L^{1-\alpha} \geq x^{1-\alpha} - \left(\frac{\epsilon \Gamma(2-\alpha)}{M} \right)$$

which means that given a numerical scheme of order $O(h^p)$ over some interval I one needs to choose a fixed memory of length L that satisfies (5.89) for all $x \in I$. This however usually means that the fixed memory is almost as large as the whole interval itself, as they point out in an example in [54].

As a result the idea of the fixed memory principle will usually not have great computational benefits. But the general idea of not sampling each point of a discretization equally still can be used to reduce the computational cost, as we will describe in the next principle.

Nested meshes and logarithmic memory principle:

After analyzing the problems of the fixed memory principle, Ford and Simpson develop the idea of nested meshes for discretized fractional derivatives in [54]. A basic idea used in [54] is to exploit the scaling property of the Riemann-Liouville fractional integral: Let $c > 0$ and f be a suitably integrable function, then

$$J^\alpha f(cx) = \int_0^{cx} (cx-t)^{\alpha-1} f(t) dt$$

and with the substitution $x = cx$

$$J^\alpha f(cx) = c^\alpha \int_0^x (x-t)^{\alpha-1} f(ct) dt.$$

Additionally for $p \in \mathbb{N}$ one gets

$$J^\alpha f(c^p x) = c^{p\alpha} \int_0^x (x-t)^{\alpha-1} f(c^p t) dt.$$

Thus any convolution weights of the convolution part of a fractional convolution quadrature can in principle be used to calculate the convolution weights for a different step size, that is

$$(5.90) \quad {}_h\Omega^\alpha f(mh) = \sum_{j=0}^m \omega_{m-j} f(jh) \Leftrightarrow {}_{c^p h}\Omega^\alpha f(c^p mh) = c^{p\alpha} \sum_{j=0}^m \omega_{m-j} f(c^p jh).$$

With this result in mind Ford and Simpson point out that one can divide a given interval $[0, X]$ non-uniformly and still obtain formulas corresponding to convolution quadratures. More precise, given a fixed memory length $L > 0$ one can decompose any given interval $[0, X]$ by

$$[0, X] = [0, X - c^q L] \cup [X - c^q L, X - c^{q-1} L] \cup \dots \cup [X - cL, X - L] \cup [X - L, X]$$

where $c \in \mathbb{N}$ and q is the smallest integer such that $X < c^{q+1}L$. In this decomposition one would use the step length h (usually used for the uniform mesh) for the most recent

interval of integration $[X - L, X]$ and successively larger step lengths over earlier intervals in the following way:

Let $X = Nh$ with some $N \in \mathbb{N}$, $X, L, h \in \mathbb{R}_+$ and $c, q \in \mathbb{N}$ such that $c^{q+1} > X \geq c^q L$. Then a fractional integral can be rewritten in the following way:

$$\begin{aligned} J_{[0,X]}^\alpha f(x) &= J_{[X-L,X]}^\alpha f(x) + \sum_{j=0}^{q-1} J_{[X-c^{j+1}L, X-c^jL]}^\alpha f(x) + J_{[0, X-c^qL]}^\alpha f(x) \\ &= J_{[X-L,X]}^\alpha f(x) + \sum_{j=0}^{q-1} c^{j\alpha} J_{[X-cL, X-L]}^\alpha f(c^j x) + c^{q\alpha} J_{[0, X-c^qL]}^\alpha f(c^q x) \end{aligned}$$

and in the discrete approximation of these integrals the convolution weights for the uniform mesh can be used converted by the scaling property (5.90). The only remaining problem might be the first interval, i.e. $[0, X - c^q L]$ which may not be an exact multiple of the current step length $c^q h$. In such a case the (short) interval can be evaluated with the step length h . In [54] Ford and Simpson showed that the described decomposition of the interval, using coarser step length in each “older” interval does not reduce the overall order of the used method, while obviously reducing the computational costs. In particular they prove

Theorem 5.5.1 *The numerical scheme indicated above preserves the order of the underlying quadrature method.*

Remark 5.5.1 *a) The fact that the singularity in the kernel of the Riemann-Liouville fractional integral occurs when $x = t$ and that $(x - t)^{\alpha-1} \rightarrow 0$ as $x \rightarrow \infty$ for $t \rightarrow 0$ suggests to distribute the computational effort logarithmically over the past, rather than uniformly.*

For example choosing $q = \lceil \log_2(X/L) \rceil$ and $c = 2$ any given step size h will remain of length h in the last two subintervals of $[0, X]$, while it will be doubled step by step for each earlier interval.

b) A detailed analysis of the reduction of the computational effort by using nested meshes and the logarithmic memory principle can also be found in [54].

Instead of simplifying the computational cost of a numerical scheme, one can try to tweak it by using already computed solutions and extrapolate them using the theory of *Richardson extrapolation* [146] as we will describe next:

Richardson extrapolation:

It is often possible to improve the performance of a numerical scheme by analyzing the error in a detailed fashion. We will show exemplary for Diethelm’s fractional backward difference method how this can be achieved. Walz and Diethelm first considered this idea in [42] and it is repeated in [33, Ch. 7.3], which we will use as basis for the following description.

To invoke Richardson extrapolation one looks for an *asymptotic expansion* of the error at a prescribed point $x_j \in [0, X]$, say, of the form

$$y(x_j) - y_j = c_1 h^{a_1} + c_2 h^{a_2} + \dots + c_M h^{a_M} + o(h^{a_M})$$

where y_j is again the approximation for $y(x_j)$ and where $0 < c_1 < c_2 < \dots < c_M$. A consequence of Theorem 5.1.7 is that, under its assumptions, $a_1 = 2 - \alpha$; the other a_j are yet to be determined. For the remainder of this section it will be useful to introduce the notation $y_h(x_j) := y_j$ for the approximation for $y(x_j)$ obtained by Diethelm's fractional backward difference method where, as usual, $x_j = jh$. This will later allow us to compare different approximations for the same value but using different step sizes. In [42, Thm. 2.1] Walz and Diethelm proved the following statement.

Theorem 5.5.2 *Let $0 < \alpha < 1$ and $f(x, y) = -\mu y + q(x)$ with some $\mu > 0$ and some function q . If the function y is sufficiently smooth, there exist coefficients c_μ and c_μ^* such that*

$$y(x_j) - y_h(x_j) = \sum_{\mu=2}^{M_1} c_\mu h^{\mu-\alpha} + \sum_{\mu=1}^{M_2} c_\mu^* h^{2\mu} + o(h^{M_3}) \quad \text{for } h \rightarrow 0$$

where M_1 and M_2 depend on the smoothness of y and $M_3 = \min\{M_1 - \alpha, 2M_2\}$.

When applying this result, it is more convenient to rearrange the two sums into just one sum.

Corollary 5.5.3 *Let $0 < \alpha < 1$ and $f(x, y) = -\mu y + q(x)$ with some $\mu > 0$ and some function q . If the function y is sufficiently smooth, there exist coefficients γ_μ such that*

$$y(x_j) - y_h(x_j) = \sum_{\mu=1}^M \gamma_\mu h^{\lambda_\mu} + o(h^{\lambda_M}) \quad \text{for } h \rightarrow 0$$

where $M = M_1 + M_2 - 1$ and, for $k = 1, 2, \dots$,

$$\lambda_{3k} = 2k + 1 - \alpha, \quad \lambda_{3k-1} = 2k \quad \text{and} \quad \lambda_{3k-2} = 2k - \alpha.$$

Remark 5.5.2 *Notice that the exponents λ_μ are explicitly given in the corollary, but the coefficients γ_μ are not. This is not a problem: We shall see that the explicit knowledge of the values of the γ_μ is not necessary in order to implement the method.*

We now explain how these results can be used to achieve our goal of improving the error: Given a point $\tau \in [0, X]$, say, we choose some initial step size h_0 such that $\tau = j_0 h_0$ with some $j_0 \in \mathbb{N}$ and calculate the approximation $y_{h_0}(\tau)$ by our algorithm. Then, we choose two additional natural numbers b and K , say, with $K \leq M$. (It is most common to choose $b = 2$.) Defining the new step sizes $h_k := h_0 / b^k$, we then calculate the new approximations $y_{h_k}(\tau)$ by the same algorithm, but this time with step size h_k , for $k = 1, 2, \dots$. Based on these approximations we then construct additional approximations by the formula

$$(5.91) \quad y_{h_k}^{(\ell)}(\tau) := \frac{b^{\lambda_\ell} y_{h_{k+1}}^{(\ell-1)}(\tau) - y_{h_k}^{(\ell-1)}(\tau)}{b^{\lambda_\ell} - 1}, \quad \ell = 1, 2, \dots, K, \quad k = 0, 1, \dots$$

with initial values

$$y_{h_k}^{(0)}(\tau) := y_{h_k}(\tau).$$

For these newly calculated values we find the following property.

Theorem 5.5.4 *Under the assumptions of Corollary 5.5.3, we have that*

$$y(\tau) - y_{h_k}^{(\ell)}(\tau) = \sum_{\mu=\ell+1}^M \gamma_{\mu}^{(\ell)} h_k^{\lambda_{\mu}} + o(h_k^{\lambda_M}) = O(h_k^{\lambda_{\ell+1}}) \quad \text{for } k \rightarrow \infty$$

(i.e. for $h_k \rightarrow 0$) with certain constants $\gamma_{\mu}^{(\ell)}$ whenever $\ell \in \{0, 1, \dots, K\}$ is fixed.

In other words, the sequence $(y_{h_k}^{(\ell+1)}(\tau))_{k=0}^{\infty}$ converges to $y(\tau)$ faster than its predecessor $(y_{h_k}^{(\ell)}(\tau))_{k=0}^{\infty}$. In addition the computation of $y_{h_0/b^k}^{(0)}$ and $y_{h_0/b^{k+1}}^{(0)}$, whose linear combination produces $y_{h_0/b^k}^{(1)}$ will in general require much less computational effort than running the algorithm with the next smaller stepsize $y_{h_0/b^{k+2}}^{(0)}$.

Richardson extrapolation similar to the one for Diethelm's fractional backward difference method are in theory possible for any of the above described numerical methods (apart from the expansion idea of Chapter 5.2) and thus can be used to improve these algorithms.

There are other mathematical ways to improve the given numerical schemes, but for now, we will end our investigation of such methods and test the described numerical methods for different examples and applications in the next chapter.

Chapter 6

Examples and applications

In this chapter we are going to investigate the numerical methods described in Chapter 5 for a number of different test problems and in addition look at their use in applications. We begin our investigation with a survey of some theoretical test equations in order to check the described analytical behaviours of the different numerical schemes.

6.1 Examples

For our first example we consider the linear fractional differential equation

$$(6.1) \quad D_*^\alpha y(x) = x^2 + \frac{2}{\Gamma(3-\alpha)} x^{2-\alpha} - y(x), \quad y(0) = 0, \quad 0 < \alpha \leq 1$$

whose exact solution is given by

$$(6.2) \quad y(x) = x^2.$$

We calculate the approximations by means of the fractional backward differentiation methods by Grünwald-Letnikov (GL), Lubich with order $p = 2$ (Lp2) and Diethelm (D) for $\alpha = 0.5$ and $\alpha = 0.1$ and various step sizes h .

The resulting errors of the different schemes at $x = 1$ are displayed in Table 6.1 for the case $\alpha = 0.5$ and in Table 6.2 for the case $\alpha = 0.1$. The notation $-5.53(-4)$ stands for $-5.53 \cdot 10^{-4}$, etc. The bottom line (marked "EOC") states the experimentally determined order of convergence for each column on the right of the table. We can see that the theoretical results of Chapter 5 hold for both tested choices of α , i.e. we get the $O(h)$, $O(h^2)$ and $O(h^{2-\alpha})$ convergence behaviour for Grünwald-Letnikov's, Lubich's and Diethelm's fractional backward difference method respectively.

In a paper by Diethelm and Walz [42] this example was solved by Diethelm's fractional backward difference methods and additionally Richardson extrapolation was performed for both choices of α . The corresponding errors of the resulting approximations at $x = 1$ are displayed in Table 6.3 and Table 6.4. According to the stated results in Chapter 5.5 the accuracy of the interpolated results improves. Additionally the experimentally determined order of convergence increases with each extrapolation.

h	Errors at $x = 1$		
	GL	Lp2	D
1/10	3.06(-2)	1.24(-3)	-7.72(-3)
1/20	1.46(-2)	3.08(-4)	-2.82(-3)
1/40	7.11(-3)	7.86(-5)	-1.02(-3)
1/80	3.51(-3)	2.01(-5)	-3.64(-4)
1/160	1.75(-3)	5.15(-6)	-1.30(-4)
1/320	8.71(-4)	1.31(-6)	-4.62(-5)
1/640	4.35(-4)	3.33(-7)	-1.64(-5)
1/1280	2.17(-4)	8.43(-8)	-5.82(-6)
1/2560	1.09(-4)	2.12(-8)	-2.06(-6)
EOC	1.00	1.99	1.50

Table 6.1: Numerical results of the three BDF schemes for equation (6.1) with $\alpha = 0.5$.

h	Errors at $x = 1$		
	GL	Lp2	D
1/10	2.74(-3)		-5.53(-4)
1/20	2.35(-3)	-4.49(-3)	-1.63(-4)
1/40	1.27(-3)	-1.10(-3)	-4.73(-5)
1/80	6.41(-4)	-2.76(-4)	-1.36(-5)
1/160	3.20(-4)	-7.07(-5)	-3.86(-6)
1/320	1.60(-4)	-1.83(-5)	-1.09(-6)
1/640	8.00(-5)	-4.75(-6)	-3.07(-7)
1/1280	3.99(-5)	-1.24(-6)	-8.57(-8)
1/2560	2.00(-5)	-3.24(-7)	-2.39(-8)
EOC	0.97	1.94	1.84

Table 6.2: Numerical results of the three BDF schemes for equation (6.1) with $\alpha = 0.1$.

Thus as a first conclusion we can ascertain that for the given linear test equation (6.1) the different low order schemes work according to their theoretical results described in Chapter 5.

Instead of carrying out further experiments on this linear example, we now turn our investigation to a nonlinear test equation, which will be more of a challenge for the numerical methods of Chapter 5.

We consider the nonlinear fractional differential equation

$$(6.3) \quad D_*^\alpha y(x) = \frac{40320}{\Gamma(9-\alpha)} x^{8-\alpha} - 3 \frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} x^{4-\alpha/2} + \frac{9}{4} \Gamma(\alpha+1) + \left(\frac{3}{2} x^{\alpha/2} - x^4 \right)^3 - y(x)^{3/2}$$

with initial condition $y(0) = 0$ for the case $0 < \alpha \leq 1$ and $y(0) = y'(0) = 0$ for the case

h_k	Errors at $x = 1$		
	$y(1) - y_{h_k}^{(0)}(1)$	$y(1) - y_{h_k}^{(1)}(1)$	$y(1) - y_{h_k}^{(2)}(1)$
1/10	-7.72(-3)		
1/20	-2.82(-3)	-1.30(-4)	
1/40	-1.02(-3)	-3.11(-5)	1.91(-6)
1/80	-3.64(-4)	-7.56(-6)	2.95(-7)
1/160	-1.30(-4)	-1.86(-6)	4.68(-8)
1/320	-4.62(-5)	-4.58(-7)	7.63(-9)
1/640	-1.64(-5)	-1.14(-7)	1.27(-9)
1/1280	-5.82(-6)	-2.82(-8)	2.14(-10)
1/2560	-2.06(-6)	-7.03(-9)	3.67(-11)
EOC	1.50	2.00	2.54

Table 6.3: Extrapolated results for equation (6.1) with $\alpha = 0.5$ using Diethelm's BDF.

h_k	Errors at $x = 1$		
	$y(1) - y_{h_k}^{(0)}(1)$	$y(1) - y_{h_k}^{(1)}(1)$	$y(1) - y_{h_k}^{(2)}(1)$
1/10	-5.53(-4)		
1/20	-1.63(-4)	-1.99(-5)	
1/40	-4.73(-5)	-4.97(-6)	1.18(-8)
1/80	-1.36(-5)	-1.24(-6)	1.47(-9)
1/160	-3.86(-6)	-3.10(-7)	1.87(-10)
1/320	-1.09(-6)	-7.75(-8)	2.43(-11)
1/640	-3.07(-7)	-1.94(-8)	3.19(-12)
1/1280	-8.57(-8)	-4.84(-9)	4.22(-13)
1/2560	-2.39(-8)	-1.21(-9)	5.60(-14)
EOC	1.84	2.00	2.91

Table 6.4: Extrapolated results for equation (6.1) with $\alpha = 0.1$ using Diethelm's BDF.

$1 < \alpha \leq 2$. The exact solution for this nonlinear fractional equation is given by

$$(6.4) \quad y(x) = x^8 - 3x^{4+\alpha/2} + \frac{9}{4}x^\alpha.$$

This time we will center our investigation around the Adams type method and Lubich's higher order fractional backward difference methods.

We first repeat the results of the Adams type method, developed in a recent paper [37]: From the solution (6.4) it follows immediately that $D_*^\alpha y \in C^2[0, 1]$ if $\alpha \leq 4$ and thus the conditions of Theorem 5.4.1 are fulfilled. In Table 6.5 the errors at $x = 1$ are shown for $\alpha = 0.25$ and $\alpha = 1.25$. Additionally the experimentally determined order of convergence is again presented in the last row. According to the theoretical results of Theorem 5.4.1 those values should be $1 + \alpha = 1.25$ for the case $\alpha = 0.25$ and 2 for the case $\alpha = 1.25$. The numerical data in the tables show that these values are reproduced approximately, at least for $\alpha = 1.25$. In the case $\alpha = 0.25$ the situation seems to be less obvious. Apparently much

smaller values for h need to be used than in the case $\alpha = 1.25$ before we can see that the asymptotic behaviour really sets in. This would normally correspond to the situation that the coefficients of the leading terms are small in magnitude compared to the coefficients of the higher-order terms.

Remark 6.1.1 *The idea of Richardson extrapolation for the Adams scheme is also discussed in [37]. Based on a conjecture [37, Conj. 3.1] on the possible error expansion for the fractional Adams scheme tests are carried out in [37]. The positive results of these tests indicate that the conjecture on the stated error expansion is valid and the performed extrapolation should in general produce good results as it did in the tests in [37].*

h	Errors at $x = 1$	
	$\alpha = 0.25$	$\alpha = 1.25$
1/10	2.50(−1)	−5.53(−3)
1/20	1.81(−2)	−1.59(−3)
1/40	3.61(−3)	−4.33(−4)
1/80	1.45(−3)	−1.14(−4)
1/160	6.58(−4)	−2.97(−5)
1/320	2.97(−4)	−7.66(−6)
1/640	1.31(−4)	−1.96(−6)
EOC	1.18	1.97

Table 6.5: Numerical results of the Adams scheme for equation (6.3).

We now carry out an extensive survey of Lubich’s fractional backward difference method of different orders for the test equation (6.3). We start with the case $\alpha = 0.5$ and check the experimental order of convergence for the cases $p = 1, \dots, 6$. We use Matlab Version 6.5 in double precision for the calculations and compare the approximate and exact solutions over various step sizes on the interval $[0, 1]$. The starting values (for the cases $p \geq 2$) are obtained by iteration and can be assumed to contain small errors. The starting weights are computed by solving the linear equation system with the Matlab backslash operator “\” (see e.g. Chapter 5.3.2). We show in Table 6.6 the errors at $x = 1$ and estimate the order of convergence for all six different methods. Additionally we present the average residuals (marked “RES”) of the starting weights computation for the smallest step size in order to analyze its influence on the behavior of the error of the different methods.

Before we draw any conclusions from Table 6.6, we need to clarify some of its entries. For $p = 5$ and $p = 6$ the largest step size(s) were not included in the calculations, since the number of starting weights are very close to, or exceed the number of overall nodes in these cases. Additionally the experimental error of convergence for $p = 5$ and $p = 6$ were computed from the non-slanted entries in the table. The slanted entries in the rows of $p = 5$ and $p = 6$ indicate some problematic behaviour, which we need to discuss in our interpretation of Table 6.6.

With these remarks in mind, we can draw several conclusions from Table 6.6. First we note that for the case $\alpha = 0.5$ the experimentally determined convergence order agrees with our theoretical results of Chapter 5.1.3 for all six choices of p . For the case $p = 5$ and $p = 6$

h	Errors at $x = 1$					
	$p = 1$	$p = 2$	$p = 3$	$p = 4$	$p = 5$	$p = 6$
1/10	-7.92(-2)	1.14(-2)	1.55(-2)	5.42(-3)		
1/20	-3.60(-2)	4.12(-3)	2.37(-3)	6.19(-4)	6.99(-5)	
1/40	-1.72(-2)	1.34(-3)	3.30(-4)	4.11(-5)	3.39(-6)	9.17(-8)
1/80	-8.43(-3)	3.67(-3)	4.34(-5)	2.63(-6)	1.10(-7)	3.07(-9)
1/160	-4.17(-3)	9.60(-5)	5.57(-6)	1.66(-7)	3.48(-9)	5.32(-11)
1/320	-2.07(-3)	2.46(-5)	7.05(-7)	1.04(-8)	1.10(-10)	1.12(-12)
1/640	-1.03(-3)	6.21(-6)	8.86(-8)	6.53(-10)	3.44(-12)	-4.19(-13)
1/1280	-5.16(-4)	1.56(-6)	1.11(-8)	4.09(-11)	9.46(-14)	-2.70(-11)
1/2560	-2.58(-4)	3.91(-7)	1.39(-9)	2.63(-12)	-4.18(-14)	-2.24(-09)
RES		1.11(-17)	1.01(-15)	6.85(-14)	3.23(-11)	2.50(-6)
EOC	1.00	2.00	3.00	3.96	4.99	5.57

Table 6.6: Numerical results of Lubich's BDF of order p for test equation (6.3) with $\alpha = 0.5$.

the numerical method exhibits problems for small step sizes, in particular we see only slight improvements by refining the step size further than a certain magnitude ($p = 5$) and even deterioration of the errors ($p = 6$). This effect is not surprising by observing the corresponding average residuals of the starting weights for these two cases, which are larger than the overall error of the methods in the problematic cases.

From our observation in Chapter 5.3 we know that the tested case $\alpha = 0.5$ is the best natured case in terms of problematic starting weights computation. In order to validate Lubich's fractional backward difference method further and for a comparison with the Adams scheme we present the numerical results for the case $\alpha = 0.25$ under the same experimental conditions as in the case $\alpha = 0.5$. The results are given in Table 6.7.

h	Errors at $x = 1$					
	$p = 1$	$p = 2$	$p = 3$	$p = 4$	$p = 5$	$p = 6$
1/10	-2.50(-1)	3.55(-2)	-2.50(-1)			
1/20	-1.79(-2)	3.34(-3)	2.69(-3)	-2.50(-1)	-4.39(-3)	
1/40	-8.56(-3)	7.18(-4)	2.69(-4)	-1.25(-4)	-4.31(-5)	-5.52(-6)
1/80	-4.25(-3)	1.77(-4)	2.81(-5)	-3.64(-6)	-1.32(-5)	-2.95(-6)
1/160	-2.10(-3)	4.46(-5)	3.25(-6)	-5.45(-6)	-6.20(-6)	-8.41(-7)
1/320	-1.04(-3)	1.13(-5)	3.89(-7)	-3.90(-6)	-1.79(-6)	6.08(-7)
1/640	-5.16(-4)	2.83(-6)	4.71(-8)	-1.40(-6)	-2.23(-6)	2.66(-7)
1/1280	-2.57(-4)	7.09(-7)	5.75(-9)	-3.73(-8)	-3.61(-6)	4.82(-4)
1/2560	-1.28(-4)	1.78(-7)	7.04(-10)	-7.99(-8)	-1.32(-4)	-2.50(-1)
RES		5.63(-16)	6.71(-12)	4.51(-7)	9.87(-5)	1.87
EOC	1.00	2.00	3.03			

Table 6.7: Numerical results of Lubich's BDF of order p for test equation (6.3) with $\alpha = 0.25$.

Again we need to address some irregularities in the presented table (Table 6.7). First we note that for the methods of theoretical order $p = 1$, $p = 3$ and $p = 4$ an error of magnitude 0.25 occurs for the widest step size. The reason for this is given by the implementation of the algorithm: The exact solution of equation (6.3) is always positive. But errors in the calculation of the numerical solution can produce a negative value at a given mesh point. In such a case the algorithm would produce a complex number for the solution at the next step since the right-hand side of (6.3) possesses a root. Therefore, the algorithm sets the numerical solution to zero for all mesh points in such a case, starting with the mesh point where a negative value was produced. Since $y(1) = 0.25$ the errors of magnitude 0.25 occur in Table 6.7 for wide step sizes.

Nevertheless, for the numerical methods of theoretical convergence order $p = 1, 2, 3$ the experimental results confirm the theoretical convergence order again. A look at the average residuals of the corresponding starting weights computations for these cases reveals that the average residual is smaller than the error produced by the corresponding numerical method in all three cases, so that we could have expected this outcome.

For the cases $p = 4$, $p = 5$ and $p = 6$ severe errors appear in the numerical results of the algorithm: As we have seen in Chapter 5.3.2 the starting weights can usually not be produced with high accuracy. As a result the corresponding residuals of the starting weights computation become large for Lubich's higher order methods as we can verify by a look at the last row of Table 6.7. This drawback has direct influence on the accuracy of the overall method as we have shown in Chapter 5.3.3 and which is also reflected in Table 6.7. In addition we can observe for the cases $p = 5$ and $p = 6$ that a refinement of the step size does not necessary imply smaller errors of the overall method, a requirement usually expected from numerical algorithms. Even worse, the algorithm breaks down for the smallest step size in the case $p = 6$ and thus produces the tabulated error of magnitude 0.25.

Furthermore we can determine that increasing the theoretical order of convergence p while not refining the step size can also result in a numerical solution, whose error becomes worse. This is something one would usually neither expect nor desire from the comparatively higher order numerical method. Summarizing, this example shows how dramatic the influence of errors in the starting weights can be. This effect becomes even more severe, because none of the usual equation system solvers produces accurate starting weights as we have determined in Chapter 5.3.2. Thus in general one has to be very careful up to which order Lubich's fractional backward difference method should be used.

A closer look at the structure of the exact solution (6.4) of the test equation (6.3) reveals that x^α is the only low order term, which theoretically needs to be compensated by the starting weights of Lubich's fractional backward difference method up to order $p = 5$. Thus the use of a reduced starting weights system, corresponding to the set $\mathcal{A} = \{0, 0.25\}$ should retain the theoretical convergence order. The results of a corresponding test under the same conditions as the last two experiments are presented in Table 6.8.

We note again that we get an error of magnitude 0.25 for $p = 2$, which can be explained as above. Furthermore for $p = 5$ we get errors close to machine precision for the two smallest step sizes, which means that the corresponding experimentally determined convergence order will be faulty. Additionally the reduced starting weight systems result in an average residual of zero for the starting weights computation in all tested cases $p = 2, \dots, 5$, meaning that the equation system is solved exactly and therefore the average residual row

h	Errors at $x = 1$			
	$p = 2$	$p = 3$	$p = 4$	$p = 5$
1/10	-2.50(-1)	5.04(-3)	3.18(-3)	1.27(-3)
1/20	1.98(-3)	1.06(-33)	2.68(-4)	4.89(-5)
1/40	6.07(-4)	1.49(-4)	1.83(-5)	1.60(-6)
1/80	1.67(-4)	1.98(-5)	1.18(-6)	5.10(-8)
1/160	4.36(-5)	2.54(-6)	7.56(-8)	1.61(-9)
1/320	1.11(-5)	3.21(-7)	4.77(-9)	5.04(-11)
1/640	2.82(-6)	4.04(-8)	2.99(-10)	1.57(-12)
1/1280	7.08(-7)	5.07(-9)	1.88(-11)	2.28(-14)
1/2560	1.78(-7)	6.35(-10)	1.21(-12)	-5.16(-14)
EOC	2.00	3.00	3.95	5.01

Table 6.8: Numerical results of Lubich's BDF of order p for test equation (6.3) with $\alpha = 0.25$ and a reduced number of starting weights corresponding to the exact solution.

("RES") in Table 6.8 is omitted.

The effect of the manipulation of used starting weights on the overall numerical method is quite powerful. The experimentally determined convergence order retains the theoretical convergence order and in addition the complexity of all four methods are almost the same. Thus the knowledge of the lower order terms in the exact solution can have great impact on the higher order fractional backward difference methods in terms of overall accuracy and complexity.

Of course, in applications one usually does not know the lower order terms in the exact solution, but we have shown in Chapter 5.2 how the asymptotic expansion can be obtained under certain conditions on the right-hand side of the fractional differential equation.

At the end of this section we want to take a closer look at the behaviour of the numerical solution based on wrongly calculated starting weights *and* starting values. We have seen in Chapter 5.3.2 that wrongly calculated starting weights may not influence the overall numerical method, if the starting values are given exactly. The following observations rest on a recent paper [35].

In Figure 6.1 we present the numerical solutions of equation (6.3) with $\alpha = 0.1$ and $p = 4$. First we use starting values obtained in the usual iterative way and then we compare this solution with one calculated using *exact* starting values. The results (shown in Figure 6.1) indicate what we have found in several examples tested for the paper [35], namely that a solution based on exact starting values may not display the same tendency to errors because of incorrect starting weights as would one based on inexact starting values. Furthermore the error at $x = 1$ produced by using exact starting values is 4.52(-7). This is about as good as the error produced by using the second order method with the same number of mesh points which is 6.05(-7) and thus the second order method would have been the more reasonable choice for this problem.

Another important drawback in the case where the starting values were obtained in the usual iterative way is that the algorithm stopped after 9850 steps since it returned a negative value at this step and thus the evaluation of the right-hand side in the next

step would produce an imaginary number as we explained above. The computation of the starting weights in Figure 6.1 were again done using the Matlab backslash operator “\”. The Matlab “gmres” function, from which we know, that it gives slightly better results, produced similar behavior when we increased the number of mesh points. For $h = 1/10\,240$ however, the algorithm finished when utilizing the GMRES algorithm and produced an error of $2.29(-6)$ at $x = 1$.

A similar effect has been observed even in the much more well-behaved case $\alpha = 0.5$ (see Figure 6.2): Here we have used the starting values obtained by perturbing the exact data by a small amount ($1(-4)$). The step size was $1/100\,000$. It turns out that in this case the numerical solution becomes negative at $x \approx 0.8$, and so the algorithm breaks down at this point. A repetition of this experiment with starting weights obtained from a high precision routine showed considerable improvements, i.e. no break down of the algorithm occurred.

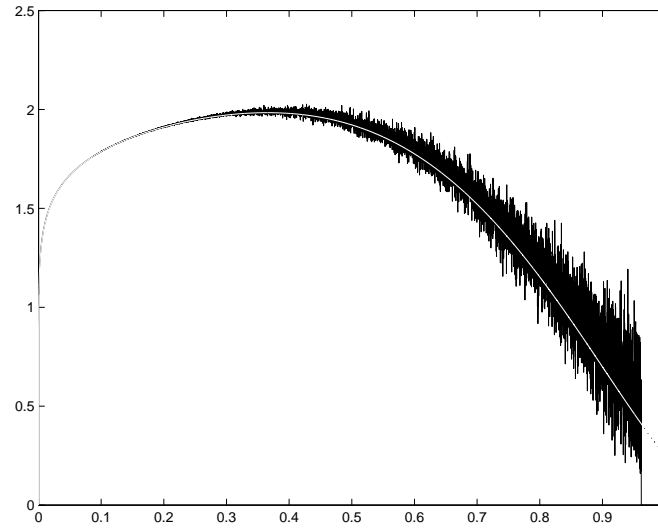


Figure 6.1: Plot of the numerical solution of example (6.3) with exact starting values (white line, dotted line) against the numerical solution with computed starting values and $\alpha = \frac{1}{10}$, $p = 4$ and $h = 1/10\,240$ (black funnel).

We have seen that the lower order numerical methods of Chapter 5 successfully work for our test problems. Lubich’s higher order fractional difference methods also produced numerical results according to the theoretical background for certain choices of α and p . But in general the higher order methods have to be used with great care because of the starting weights problem described in Chapter 5.3.2 and its influence on the overall numerical method. In particular for a given problem it might be worthwhile to try to obtain an asymptotic expansion of the exact solution to reduce the number of needed starting weights and thus the biggest drawback of the higher order methods by Lubich.

Next we are going to take a look at the possible use of the low order fractional backward difference methods for *partial* differential equations of fractional order.

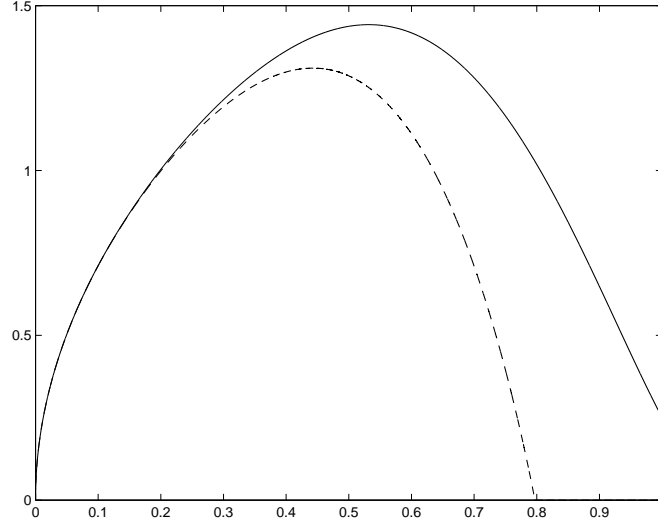


Figure 6.2: Plot of the exact solution (solid line) of example (6.3) against the numerical solution (dashed line) with parameters $\alpha = \frac{1}{2}$, $p = 4$ and $h = 1/100\,000$ and small (10^{-4}) perturbations in starting values.

6.2 Diffusion-Wave equation

Until now we have only considered ordinary differential equations of fractional order. But after some additional work the numerical methods we have described so far can also be applied to partial differential equations of fractional order. In this section we repeat ideas presented at the IFAC workshop on fractional differentiation and its applications FDA'04, see [43]:

Background of fractional diffusion-wave equations:

Standard diffusion models in one space dimension are commonly described in mathematical terms by means of the classical diffusion equation

$$(6.5) \quad \frac{\partial}{\partial t} u(x, t) + \phi(x, t) \frac{\partial^2}{\partial x^2} u(x, t) = f(x, t)$$

with given functions ϕ and f , combined with appropriate initial and boundary conditions. Most commonly one works on an interval $[a, b]$ in space and an interval $[0, T]$ in time, where T denotes the end of the time interval of interest. Typically the initial conditions in equation (6.5) are chosen as

$$(6.6) \quad u(x, 0) = u_0(x) \quad \text{for all } x \in [a, b],$$

and the boundary conditions can be of mixed Dirichlet-Neumann type,

$$(6.7a) \quad g_1(t)u(a, t) + h_1(t)\frac{\partial}{\partial x}u(a, t) = r_1(t),$$

$$(6.7b) \quad g_2(t)u(b,t) + h_2(t)\frac{\partial}{\partial x}u(b,t) = r_2(t)$$

for all $t \in [0, T]$. Here the functions $u_0, g_1, g_2, h_1, h_2, r_1$ and r_2 are assumed to be given.

It is well known that this model, which is based on Fick's law for diffusion (or on the Newton-Fourier law for heat transfer) is not always applicable. In some cases it is more appropriate to use an anomalous diffusion concept, where instead of the classical version of Fick's law, a generalized version is used, where the flow $F[u]$ induced by the field $u(x, t)$ is not only dependent on the derivative of the concentration but also on the time derivative, see e.g. [60]. One of the most obvious models in this context leads to the equation

$$(6.8) \quad D_{t,*}^\alpha u(x, t) + \phi(x, t)\frac{\partial^2}{\partial x^2}u(x, t) = f(x, t)$$

where $D_{t,*}^\alpha$ denotes Caputo's differential operator of order $\alpha \in (0, 1)$ with respect to t . Once again we use Caputo's differential operator because of its advantage with regards to the initial conditions, i.e. the fact that the initial and boundary conditions retain the form given in equations (6.6) and (6.7).

A different physical insight on the time-fractional diffusion equation can be gained by considering Brownian motion with a Random walker approach. In the classical case, advancing in time from a point t_j to t_{j+1} results in a certain jump $\pm\Delta x$ in space with a probability of $1/2$ for each case. Results usually look like the left graph in Figure 6.3. Using a generalized Brownian motion concept, where a fractional derivative in Caputo's sense of order α is used, the probability of a jump of $\pm\Delta x$ is $\alpha/2$ for each case. Additionally an earlier position x_{j+1-k} might be reached with a probability of $|\binom{\alpha}{k}|$ ($k = 2, 3, \dots, j$) or a jump back to the starting point x_0 may occur with remaining probability. The result of such a generalized Brownian motion is plotted in the right graph of Figure 6.3, see e.g. [60].

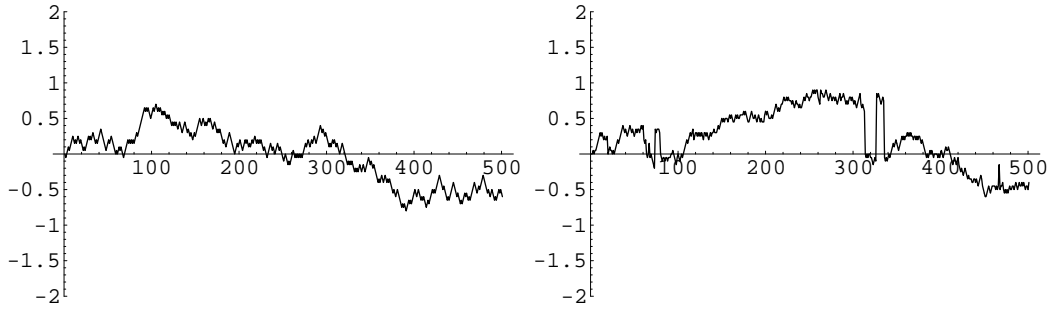


Figure 6.3: Random walker approach for Brownian motion; (l.) classical case, (r.) fractional case.

Like the classical diffusion equation, the classical wave equation

$$(6.9) \quad \frac{\partial^2}{\partial t^2}u(x, t) + \phi(x, t)\frac{\partial^2}{\partial x^2}u(x, t) = f(x, t)$$

in combination with the boundary conditions of equation (6.7) and the initial conditions of equation (6.6) and

$$(6.10) \quad u_t(x, 0) = u_1(x) \quad \text{for all } x \in [a, b],$$

can be generalized to a time-fractional version that also has the formal structure of equation (6.8), but now with $1 < \alpha < 2$, and once again we may retain the initial and boundary conditions. The result of choosing the parameter α between the two classical cases of diffusion ($\alpha = 1$) and wave equation ($\alpha = 2$) leads to a mixed behavior of diffusion and wave propagation and thus gives a direct way to describe a damped oscillation (see further Example 6.2.2).

As a result of the above argumentation, the generalized forms of both the diffusion and the wave equation may be treated in the unifying framework of the so-called *time-fractional diffusion-wave equation* (6.8), always in connection with the appropriate initial and boundary conditions. Most of the classical papers on this type of equations deal with the development of general solutions of the equation itself, but do not discuss the question of how to find solutions satisfying the given additional conditions. A notable exception is the recent paper of Agrawal [4].

Analytical expressions for the solution:

The following derivation of the analytical expression for the solution is carried out for a simplified version of the diffusion-wave equation (6.8). First of all it is possible (and usually simple) to find a function R that satisfies the boundary conditions and is twice differentiable. Then, the function $u - R$ is easily seen to fulfill an initial-boundary value problem of the same structure as the original one, only with different functions f (on the right-hand side of the differential equation) and u_0 and u_1 in the initial conditions, and with homogeneous boundary conditions. Thus it is justified to restrict the attention to the case of homogeneous boundary conditions, i.e. the case $r_1(t) = r_2(t) = 0$.

Moreover, the interval $[a, b]$ in space is assumed to be of the form $[0, L]$ with $L > 0$. This can always be achieved by a suitable affine transformation. Finally $\phi(x, t)$ is assumed to be a negative constant $-\phi$, $\phi > 0$. This is the case studied in most applications, and it will allow the construction of a very simple and elegant method for the analytic calculation of the exact solution. For the same reason the functions g_1 , g_2 , h_1 and h_2 appearing in the boundary conditions are assumed to be constant.

With these restrictions the time-fractional diffusion-wave equation can be separated into one inhomogeneous equation with homogeneous initial and boundary conditions

$$(6.11a) \quad D_{t,*}^\alpha \hat{u}(x, t) - \phi \frac{\partial^2}{\partial x^2} \hat{u}(x, t) = f(x, t),$$

$$(6.11b) \quad \hat{u}(x, 0) = 0, \quad (\hat{u}_t(x, 0) = 0),$$

$$(6.11c) \quad g_1 \hat{u}(0, t) + h_1 \frac{\partial}{\partial x} \hat{u}(0, t) = 0,$$

$$(6.11d) \quad g_2 \hat{u}(L, t) + h_2 \frac{\partial}{\partial x} \hat{u}(L, t) = 0$$

and one homogeneous equation with inhomogeneous initial and homogeneous boundary conditions

$$(6.12a) \quad D_{t,*}^\alpha \tilde{u}(x, t) - \phi \frac{\partial^2}{\partial x^2} \tilde{u}(x, t) = 0,$$

$$(6.12b) \quad \tilde{u}(x, 0) = u_0(x), \quad (\tilde{u}_t(x, 0) = u_1(x)),$$

$$(6.12c) \quad g_1 \tilde{u}(0, t) + h_1 \frac{\partial}{\partial x} \tilde{u}(0, t) = 0,$$

$$(6.12d) \quad g_2 \tilde{u}(L, t) + h_2 \frac{\partial}{\partial x} \tilde{u}(L, t) = 0,$$

where in both cases the second initial condition is only given if $\alpha \in (1, 2)$. If those two problems have been solved separately, the solution of $u(x, t)$ is the sum of $\hat{u}(x, t)$ and $\tilde{u}(x, t)$.

As in the classical case of diffusion or wave equations, the solution for (6.12) can be derived using a product approach and separation of variables for the function $\tilde{u}(x, t)$. Thus the starting point is the relation

$$\tilde{u}(x, t) = v(x)w(t)$$

with some univariate functions v and w that need to be determined. In the usual way, cf. e.g. [26, Chap. V], it is possible to construct two linear homogeneous ordinary differential equations: An equation of second order for the function v with appropriate boundary conditions derived from equations (6.12c) and (6.12d), and an equation of order α for the function w with initial conditions obtained from equation (6.12b). The former problem is exactly identical to the corresponding problem in the classical case. The only difference to the classical case is that the exponential function, which describes the basis functions of the solution space of the latter ordinary differential equation in the classical case, is replaced by the Mittag-Leffler function $E_\alpha(z)$ in the fractional case. For the sake of clarity in the following formula only Dirichlet boundary conditions are assumed to be given, i.e. h_1 and h_2 are zero in equation (6.11c), (6.11d), (6.12c) and (6.12d). The case of mixed Dirichlet-Neumann conditions can be derived in the same way but results in a more complex formula for the solution. Thus with this final simplification the solution of $\tilde{u}(x, t)$ reads

$$(6.13) \quad \tilde{u}(x, t) = \frac{2}{L} \sum_{k=1}^{\infty} E_\alpha \left(-\phi \frac{k^2 \pi^2}{L^2} t^\alpha \right) \sin \left(\frac{k\pi}{L} x \right) \int_0^L u_0(\tau) \sin \left(\frac{k\pi}{L} \tau \right) d\tau.$$

A similar reasoning for the transfer of the classical case to the fractional case for equation (6.11) leads to the solution of $\hat{u}(x, t)$, given by

$$(6.14) \quad \hat{u}(x, t) = \int_0^t \frac{2}{L} \sum_{k=1}^{\infty} E_\alpha \left(-\phi \frac{k^2 \pi^2}{L^2} (t - \xi)^\alpha \right) \int_0^L f(\tau, t) \sin \left(\frac{k\pi}{L} \tau \right) d\tau d\xi.$$

The same equations can be obtained by using the finite sine transform instead of separation of variables as shown by [4].

We know that the Mittag-Leffler function $E_\alpha(z)$ reduces for $\alpha = 1, 2$ to $E_1(-z) = \exp(-z)$ and $E_2(-z^2) = \cos(z)$, respectively. Thus the solution of equation (6.13) reads for $\alpha = 1$

$$\tilde{u}(x, t) = \frac{2}{L} \sum_{k=1}^{\infty} \exp \left(-\phi \frac{k^2 \pi^2}{L^2} t \right) \sin \left(\frac{k\pi}{L} x \right) \int_0^L u_0(\tau) \sin \left(\frac{k\pi}{L} \tau \right) d\tau$$

and for $\alpha = 2$

$$\tilde{u}(x, t) = \frac{2}{L} \sum_{k=1}^{\infty} \cos \left(\phi \frac{k\pi}{L} t \right) \sin \left(\frac{k\pi}{L} x \right) \int_0^L u_0(\tau) \sin \left(\frac{k\pi}{L} \tau \right) d\tau,$$

which represent the diffusion and wave solutions respectively. Similar arguments hold again for the equation (6.14).

Thus it is now possible to compare the classical diffusion equation ($\alpha = 1$) with its fractional counterpart ($0 < \alpha < 1$). It turns out that the only difference in the solution is that the exponential function (which is evaluated with respect to t) is replaced by the Mittag-Leffler function. The asymptotic behavior of these two functions is known to differ significantly

[58, §4]: Both functions exhibit monotonic decay to zero, but whereas the solution in the case $\alpha = 1$ decays exponentially, we only find an algebraic and hence much slower decay in the fractional situation (see also Figure 3.2). Thus, fractional diffusion takes place at a much slower speed than classical diffusion.

The wave equations can be treated in a similar way. It turns out here that the classical wave equation has sine and cosine terms, i.e. persistent oscillations, with respect to t . The fractional equation once again replaces these by Mittag-Leffler functions which now give damped oscillations up to some point T (depending on α) and then monotonic convergence to zero [58]. Thus, the fractional wave equation plays an intermediate role between classical wave and diffusion equations in that oscillations are kept alive for some time, but they are damped (i.e. information is lost).

As in the case of the classical diffusion or wave equations, the separation method can also be used for problems in more than one space dimension if the domain is a rectangle. One then simply has to set up a product with one factor for each space dimension and one factor for time, and go through the same calculations.

Numerical implementation:

Based on the analytical background we now describe a numerical method for the diffusion-wave equation (6.8), restricted to one space dimension but with arbitrary choices for the given functions in the differential equation and the initial and boundary conditions. The numerical method is based on a discretization scheme in which only a tridiagonal linear equation system needs to be solved at each time step to evaluate the discretized solution of the function $u(x, t)$.

Let $\Delta x = (b - a)/N$ and $\Delta t = T/M$ denote the step size of the discretization in the space and time axis respectively, where the values N and M are assumed to be given values defining the size of the discretization grid

$$\{x_i; t_j\}, \quad i = 0, 1, \dots, N; \quad j = 0, 1, \dots, M,$$

where $x_0 = a$ and $x_N = b$. Using the discretization on the space axis, the second derivative $u_{xx}(x, t)$ can be approximated by the central difference of second order

$$(6.15) \quad \frac{1}{\Delta x^2} \begin{pmatrix} d_1 & o_1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & o_2 & d_2 \end{pmatrix} \begin{pmatrix} u(a, t) \\ u(x_1, t) \\ \vdots \\ u(b, t) \end{pmatrix},$$

where the values d_1, o_1, o_2, d_2 are determined by the initial and boundary conditions and will be given later in this section.

Approximations of fractional derivatives are usually developed for the Riemann-Liouville derivative D_t^α as we have seen in Chapter 5.1.1 and 5.1.2 and not for the Caputo operator $D_{t,*}^\alpha$ used in the diffusion-wave equation (6.8). However by Corollary 4.1.29, both are connected by the equation

$$(6.16) \quad D_{t,*}^\alpha u(x, t) = D_t^\alpha (u - T_{[\alpha]-1}[u; 0])(x, t),$$

where $T_{[\alpha]-1}[u; 0](x, t)$ denotes the Taylor polynomial of order $[\alpha] - 1$ centered at 0. Thus by transferring the known Taylor polynomial part of (6.16) to the right-hand side of the diffusion-wave equation (6.8) any approximation of the Riemann-Liouville fractional derivative can be used. As we have seen all of these discretizations consist of a lower triangular matrix because of the non-locality of fractional derivatives. In general the discretization of $D_t^\alpha u(x, t)$ can therefore be defined by

$$(6.17) \quad \frac{1}{\Delta t^\alpha} \begin{pmatrix} \omega_{0,0} & & \\ \vdots & \ddots & \\ \omega_{M,0} & \dots & \omega_{M,M} \end{pmatrix} \begin{pmatrix} u(x, t_0) \\ \vdots \\ u(x, t_M) \end{pmatrix},$$

with some weights $\omega_{k,j}$ defined by the approximation method used. At the time-step t_k , $k = 1, \dots, M$, the values for $u(x_i, t_j)$, for $i = 0, 1, \dots, N$ and $j = 0, \dots, k-1$ are known. Thus at the time step t_k the sum

$$(6.18) \quad \sum_{v=0}^{k-1} \omega_{k,v} u(x_i, t_v), \quad i = 0, 1, \dots, N$$

can be transferred to the right-hand side of the discretization scheme as well. Therefore, at the time step t_k a tridiagonal system has to be solved, where the coefficient matrix is given by

$$\phi(x_i, t_k)A + B, \quad i = 0, 1, \dots, N.$$

Here the matrix A is defined by the discretization (6.15) and the matrix B is the matrix containing only the main diagonal of the discretization (6.17). With the above discretization the right-hand side at time step t_k is given by

$$\begin{pmatrix} r_1 \\ f(x_1, t_k) \\ \vdots \\ f(x_{N-1}, t_k) \\ r_2 \end{pmatrix} + \begin{pmatrix} 0 \\ D_t^\alpha (T_{n-1}[u; 0])(x_1, t_k) \\ \vdots \\ D_t^\alpha (T_{n-1}[u; 0])(x_{N-1}, t_k) \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ \sum_{v=0}^{k-1} \omega_{k,v} u(x_1, t_v) \\ \vdots \\ \sum_{v=0}^{k-1} \omega_{k,v} u(x_{N-1}, t_v) \\ 0 \end{pmatrix}.$$

The matrix entries d_1, o_1, o_2, d_2 and the vector entries r_1, r_2 are determined by the initial and boundary conditions using Taylor approximation. Denoting $\xi_1 = a$ and $\xi_2 = b$ they are given for $i = 1, 2$ at time step t_k by:

$$\begin{aligned} d_i &= \frac{g_i(t_k)}{\Delta x} + h_i(t_k)(-1)^i \left[\frac{1}{\Delta x^2} - \frac{\omega_{k,k}}{2\phi(\xi_i, t_k)\Delta t^\alpha} \right], \\ o_i &= (-1)^{i+1} \frac{h_i(t_k)}{\Delta x^2}, \end{aligned}$$

$$r_i = \frac{r_i(t_k)}{\Delta x} + \frac{(-1)^{i+1}h_i(t_k)}{2\phi(\xi_i, t_k)} \left[f(\xi_i, t_k) - \frac{1}{\Delta t^\alpha} \sum_{v=0}^{k-1} \omega_{k,v} u(\xi_i, t_v) + D_t^\alpha (T_{n-1}[u; 0])(\xi_i, t_k) \right].$$

In order to complete the description, we now only have to define the coefficients in the discretization of the fractional differential operator explicitly, i.e. the entries in the matrix of equation (6.17). These are directly given by our results of Chapter 5.1.1 and 5.1.2 and thus the method is completely defined. We note again that while the convergence order for the time-discretization of Diethelm's method is $O(\Delta t^{2-\alpha})$, the order of convergence for Lubich's method of first order is $O(\Delta t^\alpha)$. Thus for fractional diffusion equations, Diethelm's method is superior, while for fractional wave equations Lubich's approach is advantageous. In the following example the theoretically better suited method is used in each case.

Example 6.2.1 Consider the time-fractional diffusion problem

$$(6.19) \quad D_{t,*}^{1/2} u(x, t) - \frac{\partial^2}{\partial x^2} u(x, t) = 0$$

with the initial condition $u(x, 0) = u_0(x) = x$ and boundary conditions $u(a, t) = 0$, $u(b, t) = 1$. The solution on $[a, b] \times [0, T] = [0, 1] \times [0, 1]$ is given by $u(x, t) = x$. Both described algorithms reproduced the exact solution up to machine precision above with grid parameters $N = 67$ and $M = 80$.

Example 6.2.2 For the second example the differential equation

$$(6.20a) \quad D_{t,*}^\alpha u(x, t) - \frac{\partial^2}{\partial x^2} u(x, t) = 0$$

is solved on $[0, \pi] \times [0, 10]$ with the initial condition

$$(6.20b) \quad u(x, 0) = \sin(x), \quad u_t(x, 0) = 0$$

and boundary conditions $u(0, t) = 0$, $u(\pi, t) = 0$. This equation can either be viewed as the problem of temperature distribution in a bar generated by a point heat source kept in the middle (if $\alpha \in (0, 1)$), or (if $\alpha \in (1, 2)$) as the problem of the deflection of a string subjected to a point load at the center of the string in a string vibration setting.

In Figure 6.4 the numerical solution is plotted for the case $\alpha = 0.5$. The number of nodes in time and space were 100 and 30 respectively. In Figure 6.5 the solution for the classical version of the same diffusion problem (i.e. $\alpha = 1$) is shown for comparison. The obvious difference between those two cases is that the fractional case exhibits fast diffusion in the beginning and slow diffusion later on. If α is chosen smaller, the diffusion process over time becomes even slower. This result was to be expected because of the analytical background. In addition, in Figure 6.6 the numerical solution for $\alpha = 1.5$ is plotted, which exhibits a mixed diffusion-wave behavior. Increasing the parameter α results in an increased wave behavior, as shown in Figure 6.6, where $\alpha = 1.75$. The classical wave equation (i.e. $\alpha = 2$) is plotted in Figure 6.8 for comparison. The described behaviors were also produced by [4] for a similar problem, using only a finite sum in (6.13) as approximation to the exact solution.

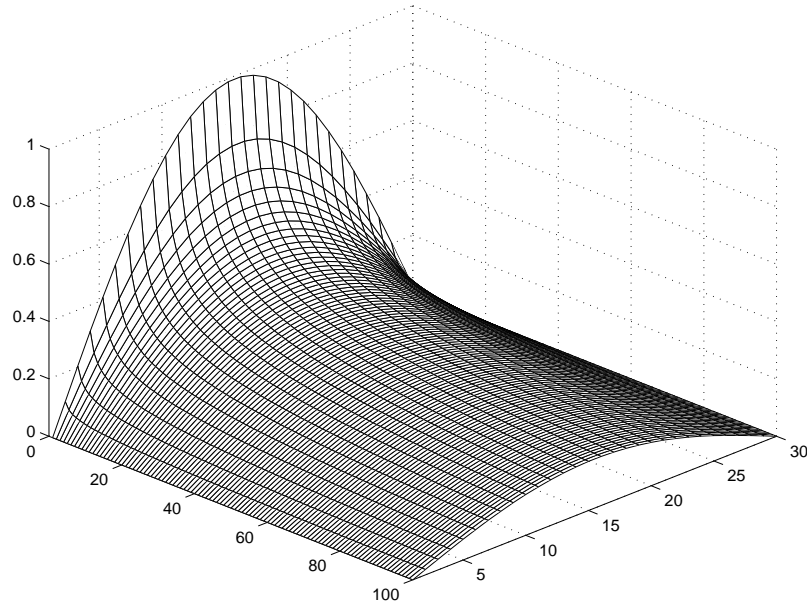


Figure 6.4: Numerical solution of equation (6.20a) for $\alpha = 0.5$.

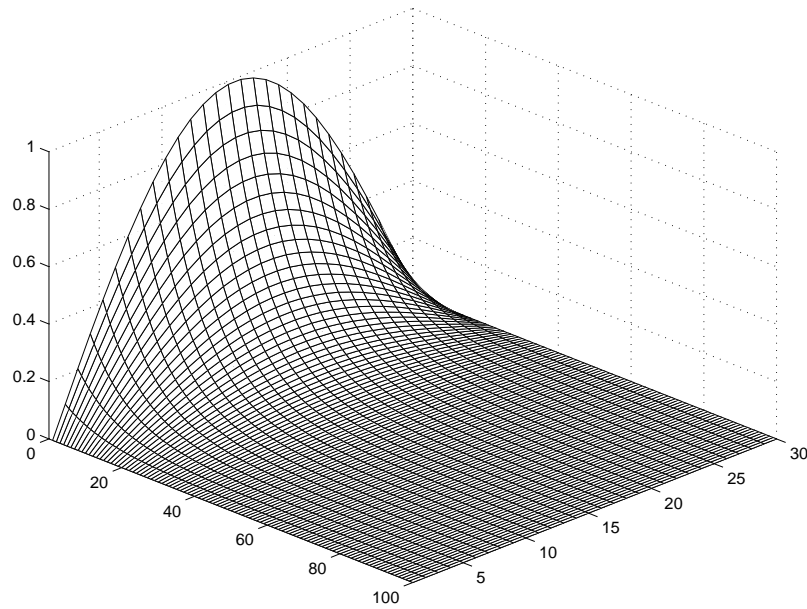


Figure 6.5: Numerical solution of equation (6.20a) for $\alpha = 1$.

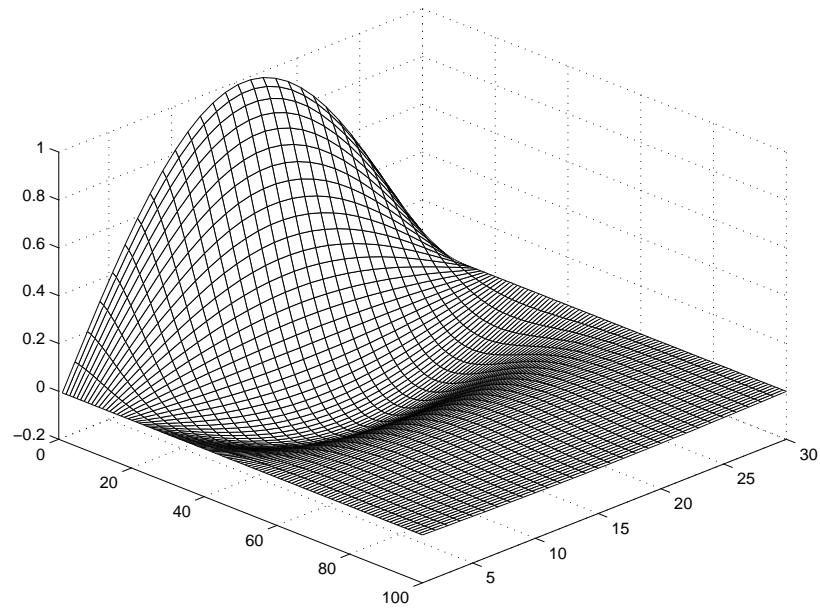


Figure 6.6: Numerical solution of equation (6.20a) for $\alpha = 1.5$.

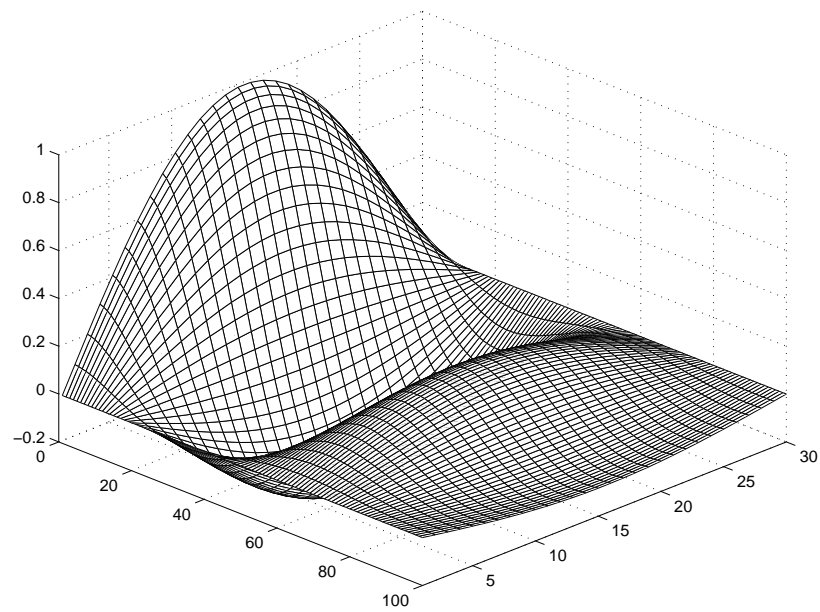


Figure 6.7: Numerical solution of equation (6.20a) for $\alpha = 1.75$.

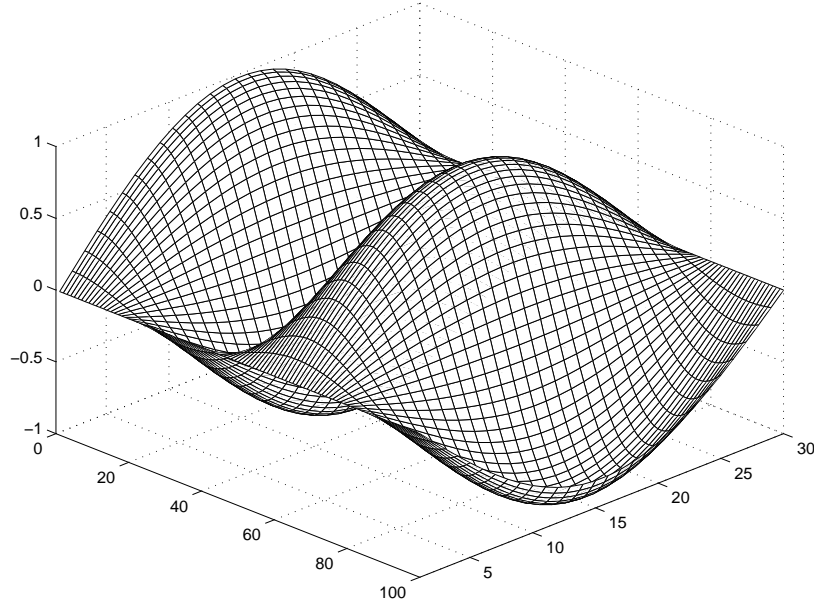


Figure 6.8: Numerical solution of equation (6.20a) for $\alpha = 2$.

We only used low order discretization schemes above, i.e. first-order methods for the derivative with respect to the time variable t and a second order scheme for the derivative with respect to the space variable x . This means that the error of the numerical solution is $O(\Delta t) + O(\Delta x)^2$. In order to achieve a higher order of convergence both of the above discretizations (6.15) and more importantly (6.17) need to be replaced by ones of higher convergence order.

A higher convergence order for the discretization in space (6.15) could be obtained by using central differences of higher order but it is known (see e.g. [70]) that additional starting values are needed then since the boundary conditions (6.7) and initial conditions (6.6), (6.10) do not give enough information to describe all matrix entries in (6.15). For a higher order discretization of the fractional derivative we would need to rely on Lubich's higher order methods, for which we know that they exhibit severe problems in an implementation.

But there are other ways to improve numerical schemes as we have indicated in Chapter 5.5. In addition we should mention that in the case $\alpha = 1$ the Crank-Nicolson scheme is very popular. It is based on a linear combination of the backward difference method described here and a corresponding forward difference method. In the fractional setting, it is possible to construct some numerical scheme that is comparable to a forward difference, but the exact leading coefficients of the error expansions are unknown at present. The knowledge of these coefficients is necessary to find the correct weights for the Crank-Nicolson scheme, and so this must remain an open question for the moment. Moreover, it is likely that the order of the second term in the error expansion in the fractional case is smaller than in the case $\alpha = 1$, and so there is reason to believe that a fractional Crank-Nicolson method (if it can be constructed) would only give a relatively small advantage

over the fractional backward difference methods used above.

So far we have taken a look at some constructed test equations and a generalization of the described numerical methods to partial differential equations of fractional order. Next we will investigate an application from physics/chemistry and in particular apply some of the described numerical methods to it.

6.3 Flame propagation¹

In this section we are going to investigate a singular problem arising in the simulation of a spherical flame initiated by a point source. This section will repeat results of a recent paper [44].

In [74] Joulin derived a model for the propagation of a flame in the context of a thermo-diffusive model with high activation energies using a gaseous mixture with simple chemistry $A \rightarrow B$. In these circumstances, he shows that the radius of the flame at time t is given by $R(t)$, where the function R is the solution of the initial value problem

$$(6.21) \quad R(t)D_*^{1/2}R(t) = R(t) \ln R(t) + Eq(t), \quad R(0) = 0.$$

The function q describes a time-dependent point source energy, and therefore it is assumed to be nonnegative, continuous and integrable on \mathbb{R}_+ , and E represents the intensity of this heat source such that $E \cdot \|q\|_{L_1(0,\infty)}$ is the total amount of energy introduced into the system.

The model described by equation (6.21) which can be justified in a mathematically rigorous way [80] has some rather natural important questions associated with it. Apart from the most obvious one for an (exact or approximate) solution for a specific choice of the parameters E and q , one is often strongly interested in the bifurcation behaviour of the equation. Analytically, the following result is known [7, Thm. 0.2]:

Theorem 6.3.1 *Assume that there exists some $t_0 > 0$ such that $q(t) > 0$ for $t \in (0, t_0)$ and $q(t) = 0$ else. Then, the initial value problem (6.21) has a unique continuous solution R . Moreover, there exists a critical value $E_{\text{crit}}(q)$ such that*

- *if $E > E_{\text{crit}}(q)$ then R is defined on $[0, \infty)$ and $\lim_{t \rightarrow \infty} R(t) = \infty$,*
- *if $E = E_{\text{crit}}(q)$ then R is defined on $[0, \infty)$ and $\lim_{t \rightarrow \infty} R(t) = 1$,*
- *if $E < E_{\text{crit}}(q)$ then there exists some finite $t_{\text{max}} > t_0$ such that R is defined on $[0, t_{\text{max}}]$ and $\lim_{t \rightarrow t_{\text{max}}} R(t) = 0$.*

Similar results can be derived in the case that the support of q is unbounded [7, Thm. 0.1]. More information on related questions may be found in [133]. From the point of view of applications however the situation discussed in Theorem 6.3.1 is by far the most relevant. Stated explicitly, it says that the flame will quench in finite time if the energy added to the system is smaller than the critical level E_{crit} , and it will burn persistently if the energy is above E_{crit} . For safety considerations it is therefore very important to find out the

¹As mentioned in the footnote of Chapter 4.3.1 newer results of the theorems in Chapter 4.3.1 have been found after this thesis was finished. In light of those results some of the results stated in this chapter will need to be reevaluated in future work on this subject

value of E_{crit} (or at least lower bounds for it) if one is interested in keeping the fire under control. On the other hand, sometimes one is interested in constructing a permanently burning flame, and then one needs to know E_{crit} (or at least upper bounds for it) in order to find an efficient process that uses as little energy as possible. Thus it is certainly justified to investigate numerical methods for the initial value problem (6.21) thoroughly. This is even more emphasized by the observation [80, p. 570] that Joulin's ideas can be carried over to a much larger class of experiments, and so one should expect that a successful algorithm for equation (6.21) will also be able to handle models from this large class too.

For our purposes it will be convenient to state the differential equation in an explicit form, i.e. we solve it for $D_*^{1/2}R$ and obtain the initial value problem in the representation

$$(6.22) \quad D_*^{1/2}R(t) = f(t, R(t)) \quad \text{with} \quad f(t, r) := \ln r + E \frac{q(t)}{r}, \quad R(0) = 0,$$

which is equivalent to the original form (6.21). Apart from the fact that this equation undergoes a bifurcation, its character introduces some additional challenges for numerical algorithms:

- The equation is singular at the origin (we shall see below that the singular contributions from the two summands on the right-hand side of equation (6.22) do not cancel each other).
- The equation is nonlinear and, what is even worse, the right-hand side does not fulfill a Lipschitz condition.

We will apply Diethelm's and Lubich's first order fractional backward difference methods to the fractional differential equation (6.22). Since this equation is singular we cannot use Lubich's fractional backward difference method of higher order in the usual fashion (since the basis functions will not have the structure as described in Corollary 4.2.8). However, the following analytical results indicate a way to increase the order of Lubich's method, which we will investigate as a third numerical method later on.

The first analytical observation deals with the asymptotic behaviour of the solution R of our problem (6.22) as $t \rightarrow 0$. It is taken from [7, Prop. 1.2].

Theorem 6.3.2 *Assume that $q(t) \geq 0$ for $t \geq 0$ and that $q(t) = q_0 t^\beta (1 + o(1))$ as $t \rightarrow 0$ with some $\beta \in [0, 1/2)$. Then, as $t \rightarrow 0$,*

$$R(t) = \rho_\beta t^{1/4+\beta/2} (1 + o(1)),$$

where

$$\rho_\beta = \left(\frac{\Gamma\left(\frac{3}{4} - \frac{\beta}{2}\right)}{Eq_0 \Gamma\left(\frac{5}{4} - \frac{\beta}{2}\right)} \right)^{1/2}.$$

Notice that this result is cited in [8, Prop. 2.1] with a factor $\sqrt{\pi}$ accidentally omitted. The significance of the condition $\beta < 1/2$ in Theorem 6.3.2 is explained by the following result taken from [7, Prop. 1.4].

Theorem 6.3.3 *Assume that $q(t) = q_0 t^\beta (1 + o(1))$ as $t \rightarrow 0$ with some $\beta \geq 1/2$. Then, as $t \rightarrow 0$,*

$$R(t) = \frac{1}{\sqrt{\pi}} t^{1/2} |\ln t| \cdot (1 + o(1)).$$

So the asymptotic behaviour of the exact solution near the origin changes as β crosses the value $1/2$.

A number of attempts have been made to construct algorithms for this problem [8, 9, 46, 74], but they typically suffer from various drawbacks. For example, Dubois and Mengué [46] report extremely long run times if a certain accuracy is desired, and the idea of Audounet et al. [9] reformulates the problem as a partial differential equation which is then treated by Fourier transform techniques, and so a certain amount of additional complexity is introduced. Therefore, it seems to be fair to say that there is a substantial demand for an efficient and well understood numerical algorithm for problems of this type.

In the classical context of first-order differential equations, it would be rather natural to use a backward differentiation formula approach for an equation with such properties. This is particularly emphasized by the fact that the initial value problem has the form

$$D_*^{1/2} R(t) = f(t, R(t)), \quad R(0) = 0,$$

with $f(0, R(0))$ being undefined. So we must find a numerical scheme that does not need to use this function value, and a backward difference method is an obvious candidate here.

As stated above we use Diethelm's and Lubich's first order fractional backward difference methods to solve the problem numerically. We start with Diethelm's formula:

Diethelm's fractional backward difference method:

For the sake of brevity we restrict our attention to a case that has turned out to be a standard example: We assume the function q that governs the energy input to have the form

$$(6.23) \quad q(t) = \begin{cases} t^{0.3}(1-t) & \text{if } 0 \leq t \leq 1, \\ 0 & \text{else.} \end{cases}$$

This problem has been considered, e.g., in [7] and [46]. In particular we will have to investigate the behaviour of the numerical solution for various choices of the total energy parameter E . One of the most important questions is of course the question for the critical value $E_{\text{crit}}(q)$. The results of Dubois and Mengué [46] appear to show that their method consistently underestimates the correct value and converges monotonically from below, with the specific result that $7.665 < E_{\text{crit}}(q)$. Moreover, their results indicate that a reasonable guess for the upper bound would be $E_{\text{crit}}(q) < 7.67$. They have used meshes with $2.5 \cdot 10^6$ mesh points to conclude these bounds.

In order to illustrate the behaviour of the numerical approximation scheme we find it most useful to display the data in such a way that we fix a step size h and calculate approximate solutions for the equation using this step size and various values of E (close to the range indicated above). A first example is shown in Figure 6.9 where we have $h = 1/20$. We see here that the critical value of this perturbed equation (the perturbation being introduced by the numerical approximation of the fractional differential operator) is between 7.796 and 7.797; so it is larger than indicated above.

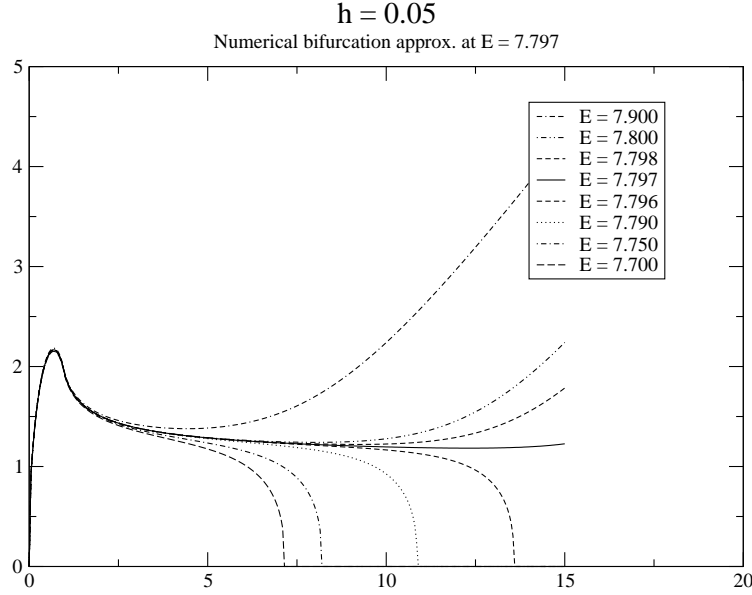


Figure 6.9: Numerical behaviour for $h = 1/20$ and various choices of E using Diethelm's fractional backward difference method.

When we successively refine the step size it turns out that the qualitative behaviour does not change, but the quantitative results move in such a way that the critical value of the perturbed equation decreases. For relatively small (but not absolutely tiny) step sizes we have been able to reproduce values similar to those of Dubois and Mengué. For $h = 1/3200$ we have concluded that the bifurcation happens between $E = 7.66549$ and $E = 7.66550$ (see Figure 6.10), and in view of the monotonicity observation this indicates that the correct value of the bifurcation parameter satisfies $E_{\text{crit}}(q) < 7.6655$. The run time of the program for such a step size was approximately 169 seconds on a 1.3 GHz Duron based PC, a value that seems to be acceptable in usual situations.

Refining the mesh even further, we can conclude the more precise bound $E_{\text{crit}}(q) < 7.665475$ (which we obtained for $h = 1/20000$). In other words, combining this upper bound with the lower bound based on the investigations of [46], we have reason to believe that $7.665 < E_{\text{crit}}(q) < 7.665475$. In particular, the combination of these two methods yields a reliable scheme for obtaining inclusions for the critical value. Moreover, the observation that the upper bound changes very little when the step size is decreased further leads to the conjecture $E_{\text{crit}}(q) = 7.66547 \pm 0.000005$.

Lubich's first order fractional backward difference method:

We consider the same restricted example as above, i.e. we assume $q(t)$ to have the form as in (6.23). First we take a closer look at the behaviour of the solution for a given total energy parameter E and different choices for the step size h . On the interval $[0, 15]$ we analyze the numerical solution for 8 different step sizes corresponding to 5000, 10000, ..., 40000 mesh points. First we consider a total energy parameter $E = 7.60$. According to the results

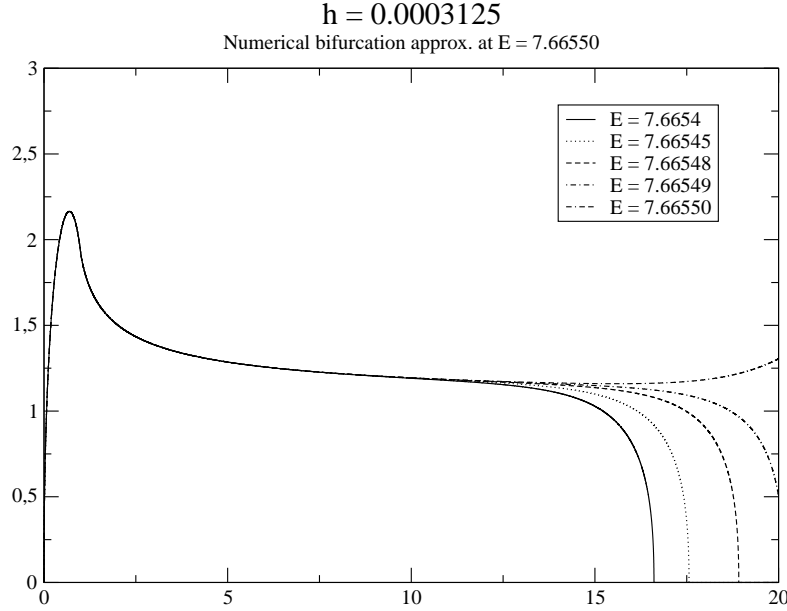


Figure 6.10: Numerical behaviour for $h = 1/3200$ and various choices of E using Diethelm's fractional backward difference method.

presented by Dubois and Mengué and confirmed using Diethelm's algorithm above, this value lies below the critical value. We can see in Figure 6.11 that we approach the exact solution from the left if we gradually reduce the step size. A similar result can be deduced if the total energy parameter is chosen above the numerically determined critical parameter. The result for $E = 7.67$ is given in Figure 6.12.

If we use again a step size of $h = 1/3200$ on the interval $[0, 20]$ Lubich's first order approach concludes that the bifurcation parameter lies between $E = 7.66705$ and $E = 7.66706$ (see Figure 6.13). In view of the monotonicity observation this indicates that the correct value satisfies $E_{\text{crit}} < 7.66706$. However we already have calculated with Diethelm's algorithm that the critical total energy lies below this value. This fact is confirmed by using a smaller step size $h = 1/20000$ for which the critical value lies between 7.6655 and 7.6656, which matches the result produced by Diethelm's fractional backward difference method.

Lubich's 'higher' order fractional backward difference method:

As we have seen in Chapter 4.2.1 the difference between regular problems and singular ones is the fact that singular problems in general do not exhibit an analytic expansion of the regular form (5.39) and thus using the starting weights of regular problems approximate the wrong basis functions in the expansion of singular problems. In order to improve the numerical method described we therefore use the weights ω of Lubich's second order fractional backward difference method and choose as additional starting weights those, who approximate the elementary functions $g_0(t) = t^0$ and $g_1(t) = t^{1/4+\beta/2}$ according to the expansion given in Theorem 6.3.2.

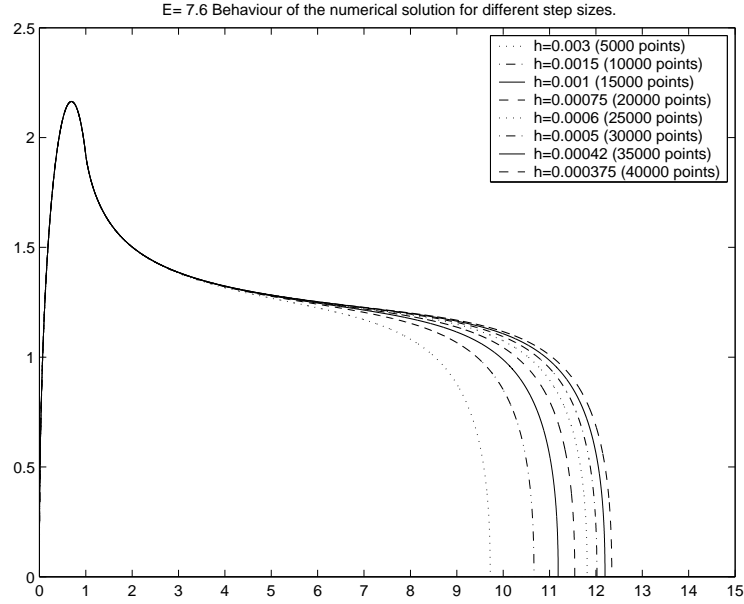


Figure 6.11: Numerical behaviour for $E = 7.60$ and various choices of h using Lubich's first order backward difference method.

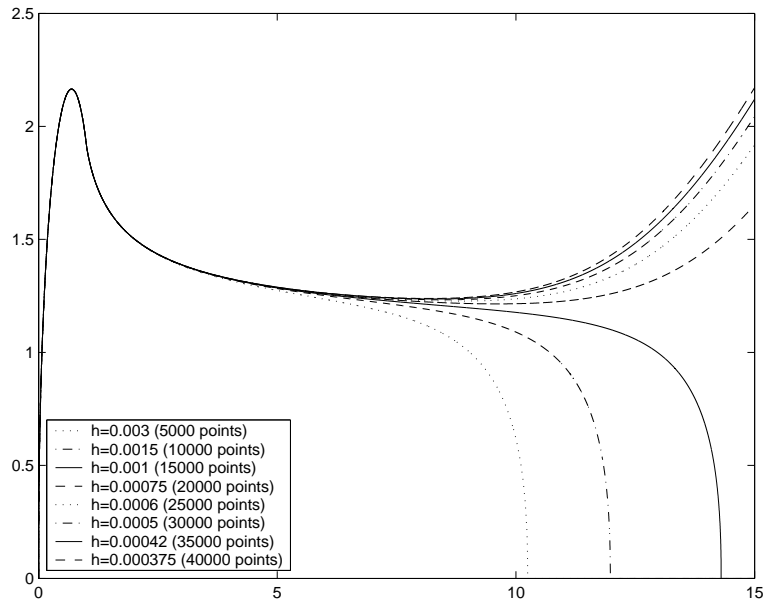


Figure 6.12: Numerical behaviour for $E = 7.67$ and various choices of h using Lubich's first order backward difference method.

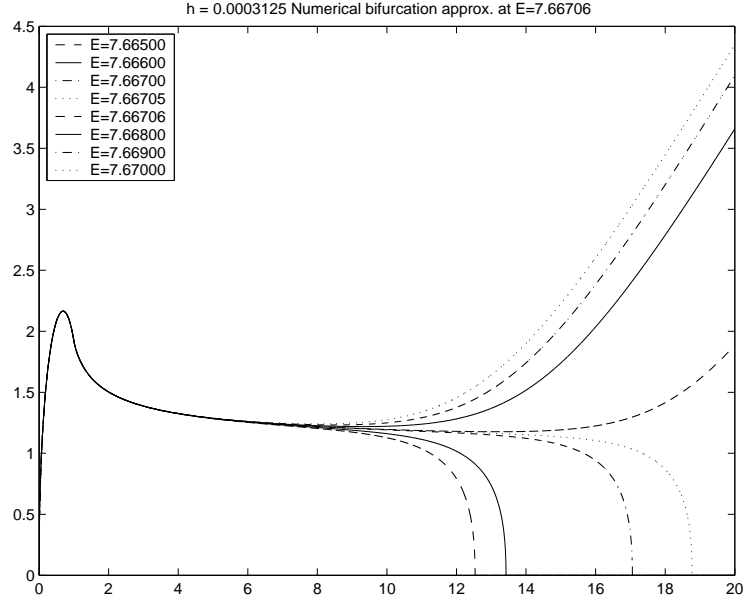


Figure 6.13: Numerical behaviour for $h = 1/3200$ and various choices of E using Lubich's first order backward difference method.

Using this modified numerical scheme with the same parameters as in the two other cases we obtain the following numerical results: By successively refining the step size for a given energy parameter E the exact solution is approached from the right (see Figure 6.14). This is a different behaviour than the other two numerical approaches presented. In view of monotonicity this means that we can gain a lower bound for the critical energy parameter instead of an upper one.

With a step size of $h = 1/1600$ on the interval $[0, 20]$ the bifurcation parameter is determined between $E = 7.663$ and $E = 7.664$ (see Figure 6.15) and thus the critical energy parameter satisfies $E_{\text{crit}} > 7.663$. Using a smaller step size $h = 1/12800$ the critical energy parameter was determined to satisfy $7.6651 < E_{\text{crit}} < 7.6652$. By refining the step size even further to $h = 1/20000$ the conjecture $E_{\text{crit}}(q) = 7.66547 \pm 0.000005$, given by Diethelm's method and supported by Lubich's first order method was reinforced.

While for the implemented higher order method a smaller number of nodes were needed to approximate the critical energy parameter, the computational costs for computing the additional starting weights reduce this advantage. Furthermore, a couple of remarks should be noted for this higher order method:

Remark 6.3.1 a) As described in the beginning of this section, Joulin's model is a singular problem and thus Lubich's fractional backward difference method of higher order cannot be applied directly. We used Theorem 6.3.2 in order to construct a higher-order numerical method. While the computations above strongly suggest that this procedure is viable, we have not proved that the numerical scheme is indeed a second order method.

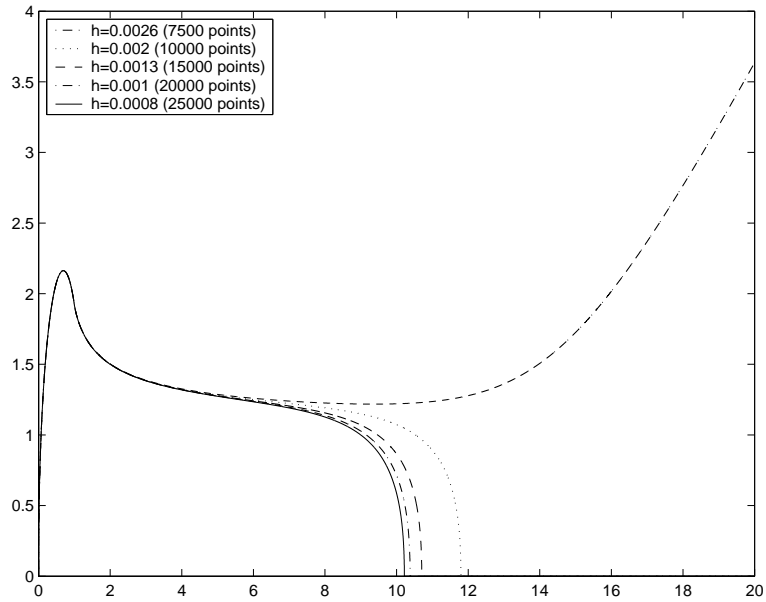


Figure 6.14: Numerical behaviour for $E = 7.65$ and various choices of h ("BDF2")

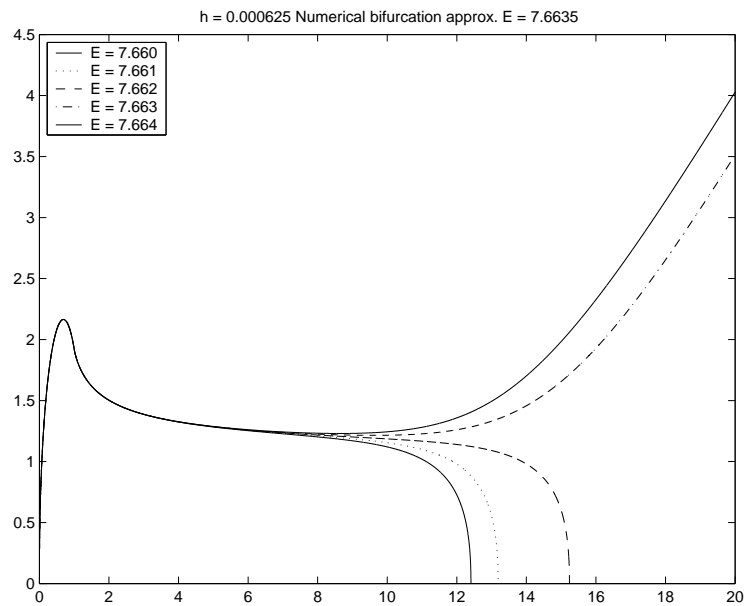


Figure 6.15: Numerical behaviour for $h = 1/1600$ and various choices of E ("BDF2")

b) The problems in computation of additional starting weights described in Chapter 5.3.2 transfer to schemes for singular problems as we carried out above.

c) The described higher order approach shows that singular problems have to be dealt with on an individual basis since there are no general expansions known for the solution of these problems. Hence in each concrete case the cost of constructing a higher order method has to be weighed up.

We note that Audounet et al. [8] have considered the slightly more general model

$$R(t)D_*^{1/2}R(t) = R(t) \ln R(t) + Eq(t) - \lambda(R(t))^3, \quad R(0) = 0,$$

which for $\lambda = 0$ reduces to our problem (6.21). With some minor modifications in the schemes used for the solution of the resulting nonlinear equations, the approaches described above can be applied to this class of problems successfully as well.

In this context we have to say that we have made use of the asymptotic expansion of the true solution (Theorem 6.3.2) in the original equation (6.22) in order to construct starting values for the Newton iteration and for the multistep methods. This type of information is not always available for a more general equation, but then we can still start the Newton iteration with an almost arbitrary positive starting value and obtain convergence. We have attempted this in connection with the above algorithms, and it turned out that the solutions typically changed by about 1 per cent in the early part ($t \leq 0.2$) and much smaller amounts later on, so the differences are insignificant. A similar observation has been made by Audounet and Roquejoffre [7, p. 25] for their method.

Chapter 7

Summary and conclusion

The structure of this thesis is conceived in such a way, that readers new to fractional calculus have an easy access to this field of mathematics. Therefore not only new results on the field of fractional calculus have been presented, but also aspects of its history (Chapter 1), important classical results (Chapters 2 and 3) and already known facts of fractional calculus (the first sections of Chapter 4). The drawback of this structure is that readers, who are not new to this mathematical field, will have greater difficulty spotting the new and significant results of this thesis. Therefore we pointed out those chapters containing new findings in the introduction. In addition we will briefly summarize those aspects of this thesis, which introduce new results in the analysis and numerics of fractional calculus below:

The first new findings can be found in Chapter 4.2.1, where analytical results on the solution of Abel-Volterra integral equations have been presented. The stated results exceed the field of fractional calculus by surveying the general class of weakly singular Volterra integral equations given by

$$(7.1) \quad y(x) = f(x) + \int_0^x (x-t)^\alpha K(x, t, y(t)) dt, \quad x \in [0, X]$$

with $\alpha > -1$ and some $X > 0$. As presented in Theorem 4.2.3 of Chapter 4.2, fractional order differential equations can be rewritten as certain Abel-Volterra integral equations and as such build a subset of the general class of the integral equations (7.1) considered in Chapter 4.2.1. The findings in that chapter consist mainly of corrections of results presented by Lubich in [94]. The first correction, presented in Theorem 4.2.7, regards the necessary assumptions on the forcing function f and the kernel K in (7.1), such that the solution y is assured to possess the form $Y(x, x^{\alpha+1})$, where $Y(z_1, z_2)$ is an analytic function. To gain this result for a non-integer order α it is necessary to assume that K is analytic in a neighbourhood of the point $(0, 0, f(0))$ and $f(x) = F(x, x^{\alpha+1})$ where $F(z_1, z_2)$ is analytic in a neighbourhood of $(0, 0)$. In [94] the basic error is the assumption that K should be analytic at the origin rather than $f(0)$. While this may only seem to be a small error, it has decisive consequences on differential equations of fractional order, since for those equations the function $f(x)$ in (7.1) is defined by the initial conditions as shown in Theorem 4.2.3. Thus only in the case of a homogeneous initial condition Lubich's erroneous result would

have no effect on the structure of the solution of a fractional order differential equation. This fact is shown in Example 4.2.1. The corrected Theorem 4.2.7 also has an interesting consequence on a different aspect of Abel-Volterra integral equations: It is commonly believed that for non-integer values α the Kernel function K cannot be smooth if the solution is smooth, and vice versa. In light of Theorem 4.2.7 we presented in Theorem 4.2.9 that the solution y is analytic if and only if $K(x, t, f(t)) = 0$ for all $x, t \in [0, X]$, given that K is analytic on a suitable set G and that f is analytic on $[0, X]$. A direct consequence of this theorem for fractional order differential equation of Caputo type, as defined in (4.24) and (4.25), is given in Corollary 4.2.11. It states that these equations have an analytic solution y if and only if $f(x, T(x)) = 0$ for all x , where T is the polynomial constructed from the initial conditions, i.e.

$$T(x) := \sum_{j=0}^{n-1} y_0^{(j)} \frac{x^j}{j!}.$$

In addition one can see that, if y is analytic then $y = T$, i.e. y is the polynomial from the kernel of the Caputo differential operator that fits the initial conditions. This result is clarified in Example 4.2.2. The rest of Chapter 4.2 rigorously extends the outlined results on the smoothness of the solution of Abel-Volterra integral equations under weaker assumptions on the differentiability of the kernel K and the forcing function f . These are also new results, which are important since in many applications, the functions under consideration have a certain number of continuous derivatives, but they are not necessarily analytic. We refrain here from repeating the results and refer to Theorems 4.2.13 and 4.2.14 and Corollary 4.2.15.

A large number of new results in the theory of fractional order differential equations can be found in various sections of Chapter 5. In those sections numerical methods for differential equations of fractional order are revised and enhanced. Some of them are tightly connected to the results of Lubich's fractional multistep methods developed in [96], which are also presented with mathematical rigour in this thesis in Chapter 4.3. Others are based on different, known and new, numerical methods. A section on known improvements of numerical methods is also included in Chapter 5 for completeness.

The first important result contained in this chapter comes again in the form of a correction of known results. In Chapter 5.1.1 a frequently used basic approach to numerically solve fractional order differential equations is presented and analyzed. A standard idea is based on the discretization of fractional order differential equation of Riemann-Liouville type

$$(7.2) \quad D^\alpha y(x) = f(x, y(x)), \quad D^{\alpha-k} y(0) = b_k \quad k = 1, 2, \dots, n-1, \quad \lim_{z \rightarrow 0+} J^{n-\alpha} y(z) = b_n$$

or Caputo type

$$(7.3) \quad D_*^\alpha y(x) = f(x, y(x)), \quad D^k y(0) = b_k \quad (k = 0, 1, \dots, n-1).$$

on a given interval $[0, X]$, for some $X > 0$ with $\alpha > 0$, $\alpha \notin \mathbb{N}$ and $n = \lceil \alpha \rceil$. The nodes of the discretization are assumed to be arranged equispaced inside the interval $[0, X]$ and on its border with a given stepsize h . Additionally the nodes are assumed to be numbered increasingly x_0, x_1, \dots, x_N , where $N = X/h$, $x_0 = 0$ and $x_N = X$. Furthermore, for the following

formulas y_m denotes the approximation of $y(x_m)$ and equally $f_m = f(x_m, y_m)$ the discretized right hand side of the differential equation in question. As standard discretization of the differential operator the finite Grünwald-Letnikov operator as defined in (4.21) is usually used.

The corrections of this basic approach are as follows: On the one hand the frequently used approach to utilize the finite Grünwald-Letnikov derivative as discretization method for either of the two given problems (7.2) and (7.3) will only work flawlessly, if homogenous initial conditions are prescribed and lead to the formula

$$(7.4) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh), \quad m = 1, \dots, N,$$

where the weights ω_k are formally given by $\omega_k = (-1)^k \binom{\alpha}{k}$. Otherwise the formula needs to be changed to

$$(7.5) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{k=1}^m \omega_k y(x_m - kh) - \left(\frac{m^{-\alpha}}{\Gamma(m-\alpha)} - \sum_{j=0}^m \omega_j \right) y_0, \quad m = 1, \dots, N,$$

and in general will only be applicable for Caputo types of fractional differential equations. On the other hand a recently published paper by Podlubny [123], which smartly solves fractional order differential equations with a matrix approach based on formula (7.4) is analyzed in Excursus 2. The analysis of this approach reveals the restriction of the method to linear problems (i.e. such problems, where the right-hand side of the differential equation is linear) and in addition a minor error of the approach as it is stated in [123] is identified. This error regards the meaning of the initial conditions in the described approach and is in detail explained in Remark 5.1.1.

The numerical methods analyzed in Chapter 5.1.1 can be understood as fractional formulation of classical backward difference methods. For this reason we also included a different approach to transfer the idea of backward difference methods to the fractional setting in Chapter 5.1.2. The presented idea is not new, in fact it was independently introduced by Chern [24] and Diethelm [31]. However, in Chapter 5.1.2 we do not only restate this approach, but also compare it with the basic approach presented in Chapter 5.1.1 and point out that they indeed differ although they both can be understood as fractional backward difference methods. The specific differences of these two methods is used in Chapter 6.2, where a new numerical method to solve partial differential equations of fractional order is presented.

In Chapter 5.1.3 we state the idea of higher order backward difference methods for fractional order differential equations. This idea is based on papers by Lubich [93, 95, 96, 97], where fractional linear multistep methods are developed for the general class of Abel-Volterra integral equations. In addition the idea was numerically implemented by Hairer, Lubich and Schlöcher in [63] for a special type of Volterra integral equations. In Chapter 5.1.3 we reformulate these results for the special case of fractional order differential equations of Caputo type. In particular Theorem 5.1.10 formulates backward difference formulas of order $p = 1, 2, \dots, 6$ for fractional differential equations of Caputo type: Given the fractional order differential equation of Caputo type (7.3), with $\alpha > 0$ and $n = \lceil \alpha \rceil$, the

backward difference formulas of order p are given by

$$(7.6) \quad y_m = h^\alpha f(x_m, y_m) - \sum_{j=0}^{m-1} \omega_{m-j} y(x_j) - \sum_{j=0}^s w_{m,j} y(x_j) + h^\alpha D^\alpha T_{n-1}[y; 0](x_m)$$

where the convolution weights ω_m are given by the generating function

$$(7.7) \quad \omega^\alpha(\zeta) = \left(\sum_{k=1}^p \frac{1}{k} (1-\zeta)^k \right)^\alpha$$

and the starting weights $\omega_{m,j}$ are given by the solution of the linear equation system

$$(7.8) \quad \sum_{j=0}^s w_{m,j} j^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)} m^{\gamma-\alpha} - \sum_{j=1}^m \omega_{m-j} j^\gamma, \quad \gamma \in \mathcal{A}$$

with \mathcal{A} defined as

$$(7.9) \quad \mathcal{A} = \{\gamma = k + j\alpha; k, j \in \mathbb{N}_0, \gamma \leq p-1\}, \quad \text{card} \mathcal{A} = s+1.$$

While this theorem is by itself only a reformulation of well known results described in Chapter 4.3, it builds the basis of one of the main results of this thesis, presented in Chapter 5.3.

Two new methods to gain an asymptotic expansion of the solution of a fractional order differential equation of Caputo type are presented in Chapter 5.2. The underlying idea of both methods is based on the idea, that the solution y of the Abel-Volterra integral equation

$$(7.10) \quad y(x) = g(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t, y(t)) dt, \quad g(x) = \sum_{k=0}^{n-1} \frac{x^k}{k!} b_k$$

corresponding to the fractional order differential equation of Caputo type can be written as a sum of simple basis terms. As additional assumption in Chapter 5.2, the problem (7.10) is assumed to be a regular initial value problem, which means that the functions $g(x)$ and $f(x, y(x))$ are assumed to possess a representation by a convergent Taylor series developed at 0 or $(0, g(0))$ respectively, i.e.

$$(7.11) \quad g(x) = \sum_{k=0}^{\infty} g_k x^k, \quad f(x, y(x)) = \sum_{\ell, m=0}^{\infty} f_{\ell, m} x^\ell (y - g_0)^m,$$

or a corresponding finite series of sufficiently high order. With the results of Theorem 4.2.7 of Chapter 4.2.1 we know that the solution y of (7.10) will exist on a certain interval $[0, X]$ and can be written as the expansion

$$(7.12) \quad y(x) = \sum_{k=0}^K \sum_{j=0}^J c_{kj} x^{k+j\alpha} + y^*(x),$$

where the parameters K and J depend on the precise smoothness properties of f and g , while y^* is smooth on $[0, X]$ and satisfies $y^*(x) = o(x^{K+J\alpha})$ as $x \rightarrow 0$.

The first method to obtain an asymptotic expansion of the exact solution of (7.10) is based on the generalization of the classical Taylor expansion approach: In this generalization the solution y in the form

$$y(x) = \sum_{j=0}^s c_j x^{\gamma_j} + y^*(x),$$

is substituted in equation (7.10) and the parameters c_j are produced by a simple formula (formula (5.41)), which is an appropriate generalization of formula (8.18) in [65, Ch. I.8] used for ordinary differential equations. The second presented approach is known as Adomian's decomposition method. It describes the asymptotic expansion as sum of basis functions $y_i(x)$, $i = 0, 1, \dots$, i.e.

$$y(x) = \sum_{i=0}^{\infty} y_i(x) = g(x) + \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} \sum_{i=0}^{\infty} {}_f A_i(t) dt,$$

where the functions ${}_f A_i(t)$ are the so called Adomian polynomials. The basis functions y_i can be determined by a simple implicit scheme (defined by equation (5.42)) based on the Adomian polynomials (5.43). In Theorem 5.2.1 we state a new simple way to compute these polynomials for the given Abel-Volterra integral equation (7.10). The two described methods are also compared in Chapter 5.2 and examples are provided, pointing out in detail the procedure of both methods.

Chapter 5.2 does not only introduce methods to compute asymptotic expansions of Abel-Volterra integral equations, but also identifies ways to simplify the computational implementation of Lubich's higher order backward difference methods introduced in Chapter 5.1.3. The question of the numerical computation of these methods is in detail analyzed in Chapter 5.3 and in particular its pitfalls are identified. A first result regards the efficient computation of the convolution weights ω_m in formula (7.6), which are defined by the generating function (7.7). Theorem 5.3.1 states that those weights can be calculated by the formula

$$(7.13) \quad \omega_m = \frac{1}{mu_0} \sum_{j=0}^{m-1} [\alpha(m-j) - j] \omega_j u_{m-j},$$

where the values u_m , $m = 0, 1, \dots$ denote the coefficients of the polynomial defining the generating function of the classical backward difference method, i.e. $\sum_{k=1}^p \frac{1}{k} (1 - \zeta)^k$. Moreover, Theorem 5.3.1 proves the validity of formula (7.13) for a broad number of linear multi-step methods and while this result is not new, the given proof uses a new idea based on automatic differentiation techniques.

The more important result of Chapter 5.3 however, is the rigorously undertaken analysis of the computation of the starting weights $w_{m,j}$ in formula (7.6). While analytically these weights are easily calculated from a regular linear equation system (7.8), we show that in practice the ill-conditioning of the given equation system prohibits in most cases the use of higher-order backward difference methods. This is shown on the one hand by carefully testing several solvers for the problematic linear equation system (including standard solvers, specially constructed solvers for the given structured coefficient matrix and

iterative solvers such as the Generalized Minimum Residual method (GMRES)), indicating that none of these produce in general results with a small residual. On the other hand the influence of the thus wrongly calculated starting weights is analyzed in detail. The result of the investigations is that higher-order backward difference methods will in general produce wrong results (unless e.g. $\alpha = 1/2$), which is shown in several examples in Chapter 6.1. However, we present in Chapter 5.3.4 how the previously developed methods of Chapter 5.2 computing the asymptotic expansion of the exact solution of fractional differential equations of Caputo type can be used to circumvent the problems of the starting weight computation. This fact is also surveyed in the examples given in Chapter 6.1.

The last two sections of Chapter 5 deal with already known results on the numerics of fractional order differential equations. In particular Chapter 5.4 states an Adams type method based on the papers [38, 39] by Diethelm and Freed. This method is stated for completeness and to compare its efficiency with the efficiency of the other presented numerical schemes in Chapter 6.1. For similar reasons Chapter 5.5 deals with several known possible improvements of the presented numerical methods. These improvements are, in parts, also considered in the examples of Chapter 6.1.

The final two new aspects presented in this thesis are of more applied nature. In Chapter 6.2 the extension of some of the presented numerical methods of Chapter 5 to the setting of partial differential equations of fractional order are considered. After a theoretical introduction to the idea and usefulness of partial differential equations of fractional order, an algorithm using the different first-order schemes of Chapter 5.1.1 and Chapter 5.1.2 is developed. This algorithm solves the type of time-fractional diffusion-wave equation given by

$$(7.14) \quad D_{t,*}^{\alpha} u(x, t) + \phi(x, t) \frac{\partial^2}{\partial x^2} u(x, t) = f(x, t)$$

where $D_{t,*}^{\alpha}$ denotes Caputo's differential operator of order $\alpha \in (0, 1)$ with respect to t . The two presented methods are tested by two different examples confirming the analytical results also contained in the chapter.

Chapter 6.3 finally deals with an problem of physics/chemistry and applies some of the presented numerical results of Chapter 5 to the given problem. More precisely, the fractional order differential equation

$$(7.15) \quad D_*^{1/2} R(t) = f(t, R(t)) \quad \text{with} \quad f(t, r) := \ln r + E \frac{q(t)}{r}, \quad R(0) = 0,$$

is analyzed. This equation is based on a flame propagation model by Joulin [74], where q describes a point source energy that depends on time, and therefore it is assumed to be nonnegative, continuous and integrable on \mathbb{R}_+ . The parameter E represents the intensity of a heat source such that $E \cdot \|q\|_{L_1(0,\infty)}$ is the total amount of energy introduced into the system. The differential equation (7.15) poses a number of complex problems for a numerical scheme. Several attempts to solve it numerically have been recently been undertaken in [8, 9, 46, 74], but they typically suffer from various drawbacks pointed out in Chapter 6.3. Therefore some of the numerical methods presented in Chapter 5 of this thesis are applied to equation (7.15) and the obtained results are compared in view of efficiency and accuracy with the earlier attempted numerical methods. The result of this comparison is that

the numerical methods presented in this thesis produce more efficient and accurate results.

The presented thesis is designed on the one hand to be an introductory work in the numerics and analysis of differential equations of fractional order. On the other hand the relatively new interest in numerical aspects of these equations permits this thesis to be more than a repetition of known results. In particular several important corrections of standard textbooks and articles on this field have been pointed out, which are quite frequently repeated in newer articles on this topic. In addition a careful analysis of the mathematical tools available to solve fractional differential equations has been undertaken in this thesis. In this context important facts of these tools have been pointed out informing engineers, as well as mathematicians, of possible complications if these tools are used and, equally important, possible workarounds if the complications are severe.

The relatively new surveyed topics in this thesis permit to point out several possible aspects, which will be needed to be investigated in further work in this field. Since most today's used numerical schemes for fractional order differential equation are basically descended from the older theory of Abel-Volterra integral equations, simplifications arising from the special structure of fractional differential equations are usually not taken into account. A first step in this direction is presented in this thesis in Chapter 5.2, where the structure of the right-hand side of a fractional differential equation is identified to have great possible impact on existing and conceivable new numerical schemes. In addition the extension of the presented results to partial and multi-term differential equation of fractional order, while already existing, is still in its infancy and possesses room for numerous improvements. Therefore, while we have seen in Chapter 1 that the field of fractional calculus is not as young as one might expect, it still has a lot of room to grow and to produce interest in the years to come.

Appendix A

List of symbols

Sets

\mathbb{N}	natural numbers, $\mathbb{N} := \{1, 2, 3, \dots\}$
\mathbb{N}_0	counting numbers, $\mathbb{N}_0 := \{0, 1, 2, \dots\}$
\mathbb{R}	real numbers
\mathbb{R}_+	positive real numbers, $\mathbb{R}_+ := \{\alpha \in \mathbb{R} : \alpha > 0\}$
\mathbb{C}	complex numbers, $\mathbb{C} := \{x + iy; x, y \in \mathbb{R}, i := \sqrt{-1}\}$
$A^n, A^n[a, b]$	set of functions with absolutely continuous derivative of order $n - 1$
$C, C[a, b]$	set of continuous functions
$C^k, C^k[a, b]$	set of function with continuous k th derivative
$H_\mu, H_\mu[a, b]$	Hölder space
$L_p, L_p[a, b]$	Lebesgue space

Functions

$E_\alpha(z)$	Mittag-Leffler function in one parameter, α
$E_{\alpha, \beta}(z)$	Mittag-Leffler function in two parameters, α, β
${}_1F_1(a; b; z)$	Kummer confluent hypergeometric function
${}_2F_1(a, b; c; z)$	Gauss hypergeometric function
$\Gamma(z)$	Euler's continuous gamma function
$B(z, w)$	Beta function in two parameters, z, w
$\ \cdot\ _\infty$	Chebyshev norm; $\ f\ _\infty = \max_{a \leq x \leq b} f(x) $
$\lceil \cdot \rceil$	Ceiling function; $\lceil x \rceil = \min\{z \in \mathbb{Z} : z \geq x\}$
$\binom{n}{k}$	Binomial coefficient; $\binom{n}{k} = n(n-1)(n-2) \cdots (n-k+1)/k!$ for $n \in \mathbb{R}$ and $k \in \mathbb{N}_0$
o, O	Landau symbols
$T_j[f, a]$	Taylor polynomial of degree j for the function f centered at the point a

Differential and Integral Operators

D^n	classical differential operator, $n \in \mathbb{N}$
J^n	Cauchy n -fold integral operator, $n \in \mathbb{N}$

D_a^α	Riemann-Liouville fractional differential operator, $\alpha \in \mathbb{R}_+$
D_{*a}^α	Caputo fractional differential operator, $\alpha \in \mathbb{R}_+$
${}^{GL}D_a^\alpha$	Grünwald-Letnikov fractional differential operator, $\alpha \in \mathbb{R}_+$
${}^{GL}_F D_a^\alpha$	Finite Grünwald-Letnikov fractional differential operator, $\alpha \in \mathbb{R}_+$
J_a^α	Riemann-Liouville fractional integral operator, $\alpha \in \mathbb{R}_+$

Integral Transforms

$\mathcal{F}f$	Fourier transform of the function f
$\mathcal{L}f$	Laplace transform of the function f

Remark: For all fractional operators the case $a = 0$ is used throughout the text with a omitted in the notation, e.g. $D_0^\alpha = D^\alpha$.

Appendix B

Some fractional derivatives

For the convenience of the reader, we provide this appendix where we give some Caputo-type derivatives with lower limit 0 of certain important functions. We do not strive for completeness in any sense, but we do want to give at least the derivatives of the classical examples.

Throughout this appendix, α will always denote the order of the Caputo-type differential operator under consideration. We shall only consider the case $\alpha > 0$ and $\alpha \notin \mathbb{N}$, and we use the notation $n := \lceil \alpha \rceil$ to denote the smallest integer greater than (or equal to) α . Recall that for $\alpha \in \mathbb{N}$, the Caputo differential operator coincides with the usual differential operator of integer order, and for $\alpha < 0$, the Caputo differential operator of negative order can be interpreted as the Riemann-Liouville differential operator of the same order. Tables of the latter are given in various places in the literature (cf., e.g., Podlubny [122] or Samko et al. [141]); we are not going to repeat those results here.

Various special functions will arise in this connection; for the precise definitions we refer to Chapter 3. By $i = \sqrt{-1}$ we denote the imaginary unit.

1. Let $f(x) = x^j$. Here we have to distinguish some cases:

$$(D_*^\alpha f)(x) = \begin{cases} 0 & \text{if } j \in \mathbb{N}_0 \text{ and } j < n, \\ \frac{\Gamma(j+1)}{\Gamma(j+1-\alpha)} x^{j-\alpha} & \text{if } j \in \mathbb{N}_0 \text{ and } j \geq n \\ & \text{or } j \notin \mathbb{N} \text{ and } j > n-1. \end{cases}$$

2. Let $f(x) = (x+c)^j$ for arbitrary $c > 0$ and $j \in \mathbb{R}$. Then

$$(D_*^\alpha f)(x) = \frac{\Gamma(j+1)}{\Gamma(j+1-n)} \frac{c^{j-n-1} x^{n-\alpha}}{\Gamma(n-\alpha+1)} {}_2F_1(1, n-j; n-\alpha+1; -x/c).$$

3. Let $f(x) = x^j \ln x$ for some $j > n-1$. Then

$$\begin{aligned} (D_*^\alpha f)(x) &= x^{j-\alpha} \sum_{k=0}^{n-1} (-1)^{n-k+1} \binom{j}{k} \frac{n!}{n-k} \frac{\Gamma(j-n+1)}{\Gamma(j-\alpha+1)} \\ &\quad + \frac{\Gamma(j+1)}{\Gamma(j-\alpha+1)} x^{j-\alpha} (\psi(j-n+1) - \psi(j-\alpha+1) + \ln x). \end{aligned}$$

4. Let $f(x) = \exp(jx)$ for some $j \in \mathbb{R}$. Then

$$(D_*^\alpha f)(x) = j^n x^{n-\alpha} E_{1, n-\alpha+1}(jx).$$

5. Let $f(x) = \sin jx$ for some $j \in \mathbb{R}$. Here again we have two cases:

$$(D_*^\alpha f)(x) = \begin{cases} \frac{j^n i (-1)^{n/2} x^{n-\alpha}}{2\Gamma(n-\alpha+1)} [-{}_1F_1(1; n-\alpha+1; ijx) \\ \quad + {}_1F_1(1; n-\alpha+1; -ijx)] & (n \text{ even}), \\ \frac{j^n (-1)^{(n-1)/2} x^{n-\alpha}}{2\Gamma(n-\alpha+1)} [{}_1F_1(1; n-\alpha+1; ijx) \\ \quad + {}_1F_1(1; n-\alpha+1; -ijx)] & (n \text{ odd}). \end{cases}$$

6. Finally we consider $f(x) = \cos jx$ with some $j \in \mathbb{R}$. As in the previous example, we obtain two cases:

$$(D_*^\alpha f)(x) = \begin{cases} \frac{j^n (-1)^{n/2} x^{n-\alpha}}{2\Gamma(n-\alpha+1)} [{}_1F_1(1; n-\alpha+1; ijx) \\ \quad + {}_1F_1(1; n-\alpha+1; -ijx)] & (n \text{ even}), \\ \frac{j^n i (-1)^{(n-1)/2} x^{n-\alpha}}{2\Gamma(n-\alpha+1)} [{}_1F_1(1; n-\alpha+1; ijx) \\ \quad - {}_1F_1(1; n-\alpha+1; -ijx)] & (n \text{ odd}). \end{cases}$$

Appendix C

Quotes

- Letter [117] from Leibniz to L'Hospital (1695):

“Vous voyés par là, Monsieur, qu’on peut exprimer par une serie infinie une grandeur comme $d^{\frac{1}{2}}\overline{xy}$, ou $d^{1:2}\overline{xy}$, quoyque cela paroisse éloigné de la Geometrie, qui ne connoist ordinairement que les differences à exposans entiers affirmatifs, ou les negatifs à l’égard des sommes, et pas encor celles, dont les exposans sont rompus. Il est vray, qu’il s’agit encor de donner $d^{1:2}x$ *pro illa serie*; mais encor cela se peut expliquer en quelque façon. Car soyent les ordonnées x en progression Geometrique en sorte que prenant une constante $d\beta$ soit $dx = xd\beta : a$, ou (prenant a pour l’unité) $dx = xd\beta$, alors ddx sera $x.\overline{d\beta}^2$, et d^3x sera $x.\overline{d\beta}^3$ etc. et $d^ex = x.\overline{d\beta}^e$. Et par cette adresse l’exposant différentiel est changé en exposant potentiel et remetant $dx : x$ pour $d\beta$, il y aura $d^ex = \overline{dx : x}^e.x$. Ainsi il s’ensuit que $d^{1:2}x$ sera egal à $x.\sqrt[2]{dx : x}$. Il y a de l’apparence qu’on tirera un jour des concequences bien utiles de ces paradoxes, car il n’y gueres de paradoxes sans utilité. Vous estes de ceux qui peuvent aller le plus loin dans les decouvertes, et je seray bientost obligé *ad lampadem aliis tradendam*. Je voudrois avoir beaucoup à communiquer, car ce vers: *Sciretuum nihil est nisi te scire hoc sciat alter*, est le plus vray en ce que des pensées qui estoient peu de chose en elles mêmes peuvent donner occasion à des bien plus belles.”

- Letter [118] from Johann Bernoulli to Leibniz (1695):

“Ex analogia potentiarum et differentiarum facile deducitur series pro $d^m\overline{xy}$ quam adducis. Interiim si m sit numerus fractus vel irrationalis, dicas mihi quaeso quid sit $d^m\overline{xy}$, an quantitas, an quid aliud? De his diu est, quod non cogitaverim, quoniam nondum ad me redii. Et difficulter a me impertrabo, ut hisce quae jam fere mihi exciderunt, de novo animum advertam. Accepi heri literas a Dno. Marchione Hospitalo, in quibus sibi eandem hanc seriem Te communicasse dicit, et simul mea, quae super hae materia me detexisse, a Te intellexerit, petit.”

- Letter [119] from Leibniz to Johann Bernoulli (1695):

“Quod quaeris de differentia, cujus exponens est fractus vel irrationalis, etiam notavi in literis ad Dnum. Marchionem Hospitalium, simulque addidi modum, per quem talis differentia potest alteri ordinariae comparari. Ex. gr. $d^{1:2}x$ sit differentia proposita. Sint x progressionis geometricae; assumpta differentiali constante dh , ut fiat $x dh : a = dx$, erit $d^2x = x dh : a = x dh dh : aa$, et similiter $d^3x = x dh^3 : a^3$, et generaliter $d^ex = x dh^e : a^e$, adeoque $d^{1:2}x = x dh^{1:2} : a^{1:2}$, seu $d^{1:2}x = x \sqrt{dh} : \sqrt{a}$ (1 : 2 mihi est idem quod $\frac{1}{2}$; et $dh : a$ idem quod $\frac{dh}{a}$). Unde vides talium differentiarum valores hoc modo haberi posse per radicem vel potentiam ordinariae differentiae. Quod cum memorabile sit, Tibi non ingratum fore puto. Easdem extraordinarias differentias per seriem infinitam ex ordinariis conflata exprimi posse, me non monente, vides, adeoque suo modo reales esse, etiam hinc patet.”

- Letter [120] from Leibniz to J. Walis (1697):

“Mihi consideratio Differentiarum et Summarum in seriebus Numerorum primam lucem affuderat, cum animadverterem differentias tangentibus, et summas qaadraturis respondere. Vidi mox differentias differentiarum in Geometria osculis exprimi, et notavi mirabilem analogiam relationis inter differentias et summas cum relatione inter potentias et radices. Itaque judicavi, praeter affectiones quantitatis hactenus receptas $y, y^2, y^3, y^{\frac{1}{2}}, y^{\frac{1}{3}}$ etc, vel generaliter y^e , sive $\boxed{p^e}y$, vel potentiae ipsius y secundum exponentem e , posse adhiberi novas differentiarum vel fluxionum affectiones dy, d^2y (seu ddy), d^3y (seu ddy), imo utiliter etiam occurrit $d^{\frac{1}{2}}y$, et similiter generaliterque d^ey .”

- Paper [52] by Leonhard Euler (1716):

“27. Coronidis loco adhuc aliquid, curiosum id quidem magis quam utile, adiungam. Notum est per $d^n x$ intelligi differentiale ordinis n ipsius x et $d^n p$, si p denotet functionem quampiam ipsius x ponaturque dx constans, esse homogeneum cum dx^n ; semper autem, quando n est numerus integer affirmativus, ratio, quam habet $d^n p$ ad dx^n , algebraicae potest exprimi; ut si $n = 2$ et $p = x^3$, erit $d^2(x^3)$ ad dx^2 ut $6x$ ad 1. Quaeritur nunc, si n sit numerus fractus, qualis tum futura sit ratio. Difficultas in hisd casibus facile intelligitur; nam si n est numerus integer affirmativus, $d^n x$ continua differentiatione invenitur; talis autem via non patet, si n est numerus fractus. Sed tamen ope interpolationum progressionum, de quibus in hac dissertatione explicavi, rem expedire licebit.”

- Book [78] by P. S. Laplace (1812):

“On voit par ce qui précède, l’analogie qui existe entre les fonctions génératrices des variables, et les intégrales définies au moyen desquelles ces variables

peuvent être exprimées. Pour la rendre encore plus sensible, considérons l'équation

$$y_x = \int T.dt.t^{-x},$$

T étant une fonction de t , et l'intégrale étant prise dans des limites déterminées. On aura, x variant de α

$$\Delta.y_x = \int T.dt.t^{-x} \cdot \left(\frac{1}{t^\alpha} - 1 \right)$$

et généralement

$$\Delta^i.y_x = \int T.dt.t^{-x} \cdot \left(\frac{1}{t^\alpha} - 1 \right)^i;$$

en faisant i négatif, la caractéristique Δ se change dans le signe intégral Σ . Si l'on suppose α infiniment petit et égal à dx ; on aura $\frac{1}{t} = 1 + dx \cdot \log \frac{1}{t}$; on aura donc, en observant qu'alors $\Delta^i.y_x$ se change dans $d^i.y_x$,

$$\frac{d^i.y_x}{dx^i} = \int T.dt.t^{-x} \cdot \left(\log \frac{1}{t} \right)^i.$$

On trouvera de la même manière, et en adoptant les dénominations du n° 2,

$$\nabla^i.y_x = \int T.dt.t^{-x} \cdot \left(a + \frac{b}{t} \dots + \frac{q}{t^n} \right)^i.$$

Ainsi la même analyse qui donne les fonctions génératrices des dérivées successives des variables, donne les fonctions sous le signe \int , des intégrales définies qui expriment ces dérivées. La caractéristique ∇^i n'exprime, à proprement parler, qu'un nombre i , d'opérations consécutives; la considération des fonctions génératrices réduit ces opérations à des élévations d'un polynôme à ses diverses puissances; et la considération des intégrales définies donne directement l'expression de $\nabla^i.y_x$, dans le cas même où l'on supposerait i un nombre fractionnaire. [...]

Lorsqu'une fonction y_s de s peut être exprimée par une intégrale définie de la forme $\int x^s \cdot \varphi dx$, les différences infiniment petites et finies d'un ordre quelconque n , seront par le n° 21,

$$\begin{aligned} \frac{d^n.y_s}{ds^n} &= \int x^s \cdot \varphi dx \cdot (\log x)^n, \\ \Delta^n.y_s &= \int x^s \cdot \varphi dx \cdot (x - 1)^n. \end{aligned}$$

Si au lieu d'exprimer la fonction de s , par l'intégrale $\int x^s \cdot \varphi dx$, on l'exprime par l'intégrale $\int c^{-sx} \cdot \varphi dx$, alors on a

$$\begin{aligned} \frac{d^n.y_s}{ds^n} &= (-1)^n \cdot \int x^n \cdot \varphi dx \cdot c^{-sx}, \\ \Delta^n.y_s &= \int \varphi dx \cdot c^{-sx} \cdot (c^{-x} - 1)^n. \end{aligned}$$

Pour avoir les intégrales n^{iemes} , soit finies, soit infiniment petites, il suffira de faire n négatif dans ces expressions. On peut observer qu'elles sont généralement vraies, quel que soit n , en le supposant même fractionnaire; ce qui donne le moyen d'avoir les différences et les intégrales correspondantes à des indices fractionnaires. Toute la difficulté se réduit à mettre sous la forme d'intégrales définies, une fonction de s ; ce que l'on peut faire par les nos 29 et 30, lorsque cette fonction est donnée par une équation linéaire aux différences infiniment petites ou finies. Comme on est principalement conduit dans l'analyse des hasards, à des expressions qui ne sont que les différences finies des fonctions, ou une partie de ces différences; nous allons y appliquer les méthodes précédentes, et déterminer leurs valeurs en séries convergentes.

- Book [76] by S. F. Lacroix (1819):

“Au moyen des intégrales définies, Euler parvient encore à une interpolation très-digne de remarque, c'est celle des fonctions différentielles. De même qu'entre les puissances entières, on insère, par l'extraction des racines, des puissances fractionnaires, de même aussi l'on peut concevoir des termes intermédiaires dans la serie

$$V, \quad dV, \quad d^2V, \quad d^3V, \dots d^nV,$$

des différentielles d'une même fonction, et désigner ces termes par un indice fractionnaire qui marque le rang qu'il occupent dans la série proposée. Il ne sera pas plus possible d'interpréter ces quantités par des différentiations successives, que d'expliquer les puissances fractionnaires par des multiplications répétées; mais les formules $d^{\frac{1}{2}}V$ et $V^{\frac{1}{2}}$ seront des expressions formées par analogie, l'une dans la série des différentielles, l'autre dans celles des puissances.

Soit, pour exemple, $V = v^m$; lorsque n est un nombre entier, on a, quelle que soit m ,

$$d^n(v^m) = m(m-1) \dots (m-n+1)v^{m-n}dv^n = \frac{[m]^m}{[m-n]^{m-n}}v^{m-n}dv^n;$$

mettant pour $[m]^m$ et $[m-n]^{m-n}$ les expressions données par la formule du n° 1160, on trouvera

$$d^n(v^m) = v^{m-n}dv^n \frac{\int dx (1/\frac{1}{x})^m}{\int dx (1/\frac{1}{x})^{m-n}}.$$

C résultat est susceptible d'une vérification immédiate, en s'assurant qu'il rentre dans ceux que l'on connaît les cas où n est un nombre entier positif.

Si l'on fait $m = 1$, $n = \frac{1}{2}$, il viendra

$$d^{\frac{1}{2}}v = \sqrt{v}dv \frac{\int dx 1/\frac{1}{x}}{\int dx (1/\frac{1}{x})^{\frac{1}{2}}} = \frac{\sqrt{v}dv}{\frac{1}{2}\sqrt{\pi}},$$

en observant qu'entre les limites 0 et 1,

$$\int dx 1 \frac{1}{x} = 1, \quad \int dx \left(1 \frac{1}{x}\right)^{\frac{1}{2}} = \left[\frac{1}{2}\right]^{\frac{1}{2}} = \frac{1}{2}\sqrt{\pi},$$

π étant la demi-circonférence du cercle dont le rayon est 1 (1160).

C'est ainsi que l'on parviendrait à l'équation primitive de la courbe correspondante à l'équation différentielle

$$y d^{\frac{1}{2}}v = v \sqrt{dy},$$

dans laquelle dv est supposée constante. Au moyen de la valeur précédente de $d^{\frac{1}{2}}v$, on la transformerait d'abord en $\frac{y\sqrt{v}dv}{\frac{1}{2}\sqrt{\pi}} = v\sqrt{dy}$; et quarrant ensuite chacun de ses membres, on obtiendrait $\frac{v^2 dv}{\frac{1}{4}\pi} = v dy$, d'où l'on conclurait

$$\frac{1}{\frac{1}{4}\pi} 1v = C - \frac{1}{y}, \quad \text{ou} \quad y 1v = \frac{1}{4}C\pi y - \frac{1}{4}\pi."$$

- Book [56] by J. B. J. Fourier (1822):

"Nous ferons aussi remarquer que l'on peut déduire de l'équation (B) une expression très-simple du coefficient différentiel de l'ordre indéfini $\frac{d^i}{dx^i}fx$, ou de l'intégrale $\int^i dx^i.fx$.

L'expression cherchée est une certaine fonction de x et de l'indice i . Il s'agit de connaître cette fonction sous une forme telle, que le nombre i n'y entre point comme indice, mais comme une quantité, afin de comprendre, dans une même formule, tous les cas où l'on attribue à i des valeurs positives ou négatives quelconques. Pour y parvenir, nous remarquerons que l'expression $\cos.(r + i\frac{\pi}{2})$, ou

$$\cos.r.\cos.\left(\frac{i\pi}{2}\right) - \sin.r.\sin.\left(\frac{i\pi}{2}\right),$$

devient successivement

$$-\sin.r, -\cos.r, +\sin.r, +\cos.r, -\sin.r, \dots \text{etc.},$$

si les valeurs respectives de i sont 1, 2, 3, 4, 5, etc. Les mêmes résultats reviennent dans le même ordre, lorsqu'on augmente la valeur de i . Il faut maintenant, dans le second membre de l'équation

$$fx = \frac{1}{2\pi} \int d\alpha f\alpha \int dp \cos.(px - p\alpha),$$

écrire le facteur p^i au-devant du signe cosinus, et ajouter sous ce signe le terme $+ \frac{i\pi}{2}$. On aura ainsi

$$\frac{d^i}{dx^i}fx = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\alpha f\alpha \int_{-\infty}^{+\infty} dp.p^i.\cos(px - p\alpha + i\frac{\pi}{2}).$$

Le nombre i , qui entre dans le second membre, sera regardé comme une quantité quelconque positive ou négative. Nous n'insisterons point sur ces applications à l'analyse générale;"

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Summary

Efficient numerical methods for fractional differential equations and their theoretical background are presented. A historical review introduces and motivates the field of fractional calculus. Analytical results on classical calculus as well as special functions and integral transforms are repeated for completeness. Known analytical results on non-integer order differentiation and integrations are presented and corrected and extended where needed. On those results several numerical methods for the solution of fractional differential equations are based. These methods are described and compared to each other in detail. Special attention is paid to the question of applicability of higher order methods and in connection the practical implementation of such methods is analyzed. Different ways of improvements of the presented numerical methods are given. Numerical calculations confirm the results which were deduced theoretically. Moreover, some of the presented methods are generalized to deal with partial differential equations of fractional order. Finally a problem of physics/chemistry is presented and some of the presented numerical methods are applied.

Zusammenfassung

Effiziente numerische Methoden für fraktionale Differentialgleichungen und ihr theoretischer Hintergrund werden betrachtet. Ein historischer Rückblick liefert eine Einführung und Motivation in das Gebiet der fraktionalen Differential- und Integralrechnung. Analytische Ergebnisse der klassischen Differential- und Integralrechnung, sowie spezielle Funktionen und Integraltransformationen werden zur Vollständigkeit wiederholt. Bekannte analytische Ergebnisse nicht-ganzzahliger Differentiation und Integration werden dargelegt und berichtigt und erweitert falls nötig. Auf diesen Ergebnissen beruhen mehrere numerische Methoden für die Lösung fraktionaler Differentialgleichungen. Diese Methoden werden detailliert beschrieben und untereinander verglichen. Besonderer Wert wird auf die Frage nach der Anwendbarkeit der Methoden höherer Ordnung gelegt und in diesem Zusammenhang die praktische Implementierung solcher Methoden untersucht. Verschiedene Möglichkeiten zur Verbesserung der beschriebenen Methoden werden vorgestellt. Numerische Berechnungen bestätigen die theoretisch hergeleiteten Ergebnisse. Des Weiteren werden einige der vorgestellten Methoden verallgemeinert, um auf partielle Differentialgleichungen fraktionaler Ordnung angewendet werden zu können. Letzlich wird ein Problem aus der Physik/Chemie vorgestellt und einige der dargestellten numerischen Methoden darauf angewendet.